AUG 4 1988 501-G-34 HE20.3180/2:988

COMPLETED

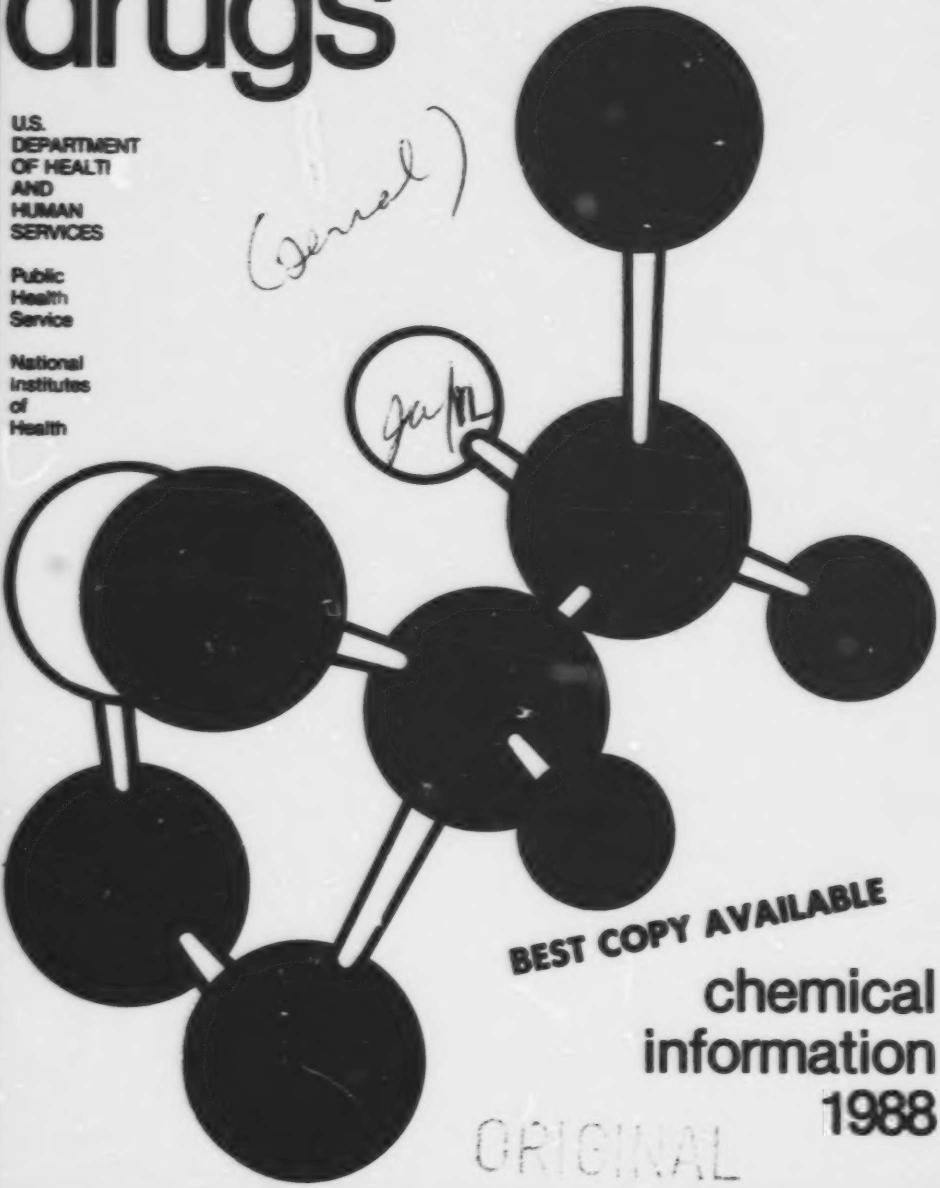
nci investigational drugs

U.S.
DEPARTMENT
OF HEALTH
AND
HUMAN
SERVICES

Public
Health
Service

National
Institutes
of
Health

(Serial)



BEST COPY AVAILABLE

chemical information 1988

ORIGINAL

nci investigational drugs

chemical information

U.S.
DEPARTMENT
OF HEALTH
AND
HUMAN
SERVICES

Public
Health
Service

National
Institutes
of
Health

NIH Publication
No. 88-2654
August 1988

PREFACE

NCI Investigational Drugs - Chemical Information has been prepared by the Pharmaceutical Resources Branch, Developmental Therapeutics Program, Division of Cancer Treatment, National Cancer Institute. The chemical information presented was obtained from National Cancer Institute contractors. The following organizations and individuals contributed to the preparation of this book:

Developmental Therapeutics Program
National Cancer Institute

Karl P. Flora	James C. Cradock
Frank R. Quinn	J. Paul Davignon
G.W.A. Milne	Larry M. Kleinman
Valerie A. Damiano	Janet M. Morgan
Lawrence A. Trissel	B. Rao Vishnuvajjala

ORI, Inc.
Bethesda, Maryland

Donald A. Koss, Jr.

Midwest Research Institute
Kansas City, Missouri

Evelyn Murrill	Mary Valla Crook
Nita West	Andrea Schierhoff
Gene Ray	Tim Skinner

Research Triangle Institute
Research Triangle Park, North Carolina

John W. Hines
Kenneth H. Davis, Jr.
Patricia A. Blau
Andy McDaniel
Donna L. Scott
David T. Nuttall

SRI International
Menlo Park, California

Peter Lim
Andrew Cheung
Mechelle Carnine
Carol Carlson
Yvette Ha
Donna Hawkins
Deborah Kenney
Lori Olson
Karl Sackinger
Elaine Shingai Struble
Nahid Vidensek

This document was prepared using the Centrum technical information management system, provided by the Polygen Corporation, Waltham, Massachusetts.

Other contributers are listed in the Previous (1984) edition.

Copies of this publication may be requested by writing to the following address:

Pharmaceutical Resources Branch
National Cancer Institute
Executive Plaza North, Room 818
Bethesda, Maryland 20892

INTRODUCTION

NCI Investigational Drugs - Chemical Information is designed to provide selected relevant chemical and physical data to investigators involved in various multidisciplinary studies of drugs which were developed or are being developed by the Developmental Therapeutics Program, Division of Cancer Treatment, National Cancer Institute. Monographs are presented on most of the investigational agents currently distributed by the Division of Cancer Treatment for clinical study. Monographs are also presented for many compounds in preclinical development.

Selected chemical information is presented in a standardized format to facilitate the retrieval of specific information. The format includes the chemical name, common names, molecular formula, molecular weight and structure of each compound. Generally, approximate solubility, stability, ultraviolet absorption, and chromatographic information is provided. Occasionally other selected data are provided (e.g. optical rotation).

The approximate solubility data are generated during the early stages of drug development. These studies are not necessarily conducted under "saturation conditions" and are intended only to provide rough solubility estimates for guidance during the formulation development process. As such, they should be useful for providing leads such as the potential suitability of a particular solvent as a vehicle for animal studies or for use in extracting the drug from biological fluids.

The bulk drug stability data provided are also generated early in the development process. These studies are intended to identify potential stability problems as well as identify a possible stable storage condition for the bulk drug. The data are not intended to support long term stability during storage. They can, however, be used as a general guide as to the relative stability of the bulk drug. The solution stability data may provide guidance as to the storage of solutions prepared from bulk drug (e.g. some solutions may need to be prepared immediately before use).

Data from some analytical testing are presented as a range of values. These ranges are derived from the assay of multiple bulk drug samples and are typical of the values that were generated from the better samples received for analysis. Unless otherwise indicated, samples are assayed on an "as is" basis. Corrections for water content are not generally applied.

The chromatographic procedures provided [usually high performance liquid chromatographic (HPLC) procedures] are those which were developed by the analytical contractors and have been used for the assay of multiple lots of bulk drugs and clinical drug products. As such, the methods may not be immediately useful for other applications. For example, the inclusion of an extraction/isolation step or a change in detection mode may be necessary to allow the quantitation of drug in biological fluids. However, the methods can provide a starting point for developing these more specialized procedures thus eliminating some of the time spent on methods development. It should be noted that the HPLC columns listed in the method description are the actual columns used in our analyses of the material. This is not to imply that other similar columns will not perform as well or perhaps better. Also, it should be recognized that the transfer of HPLC methodology from laboratory to laboratory will likely require some amount of "fine tuning" and that retention volumes and other chromatographic characteristics may not be identical for a given set of operating conditions.

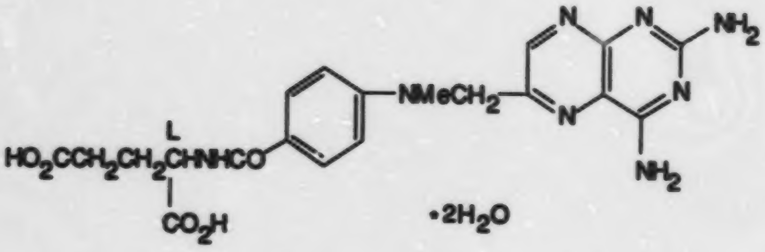
Toxicity data were derived from the Registry of Toxic Effects of Chemical Substances compiled by the National Institute of Occupational Safety and Health, the Toxicology Branch (NCI) and *in vivo* screening data (NCI). These data are provided for general guidance only and no warranty of accuracy is implied by their inclusion. Further information should be obtained from the primary source.

Additional analytical chemistry information is available upon request from the Pharmaceutical Resources Branch, National Cancer Institute.

For information on the pharmaceutical dosage forms refer to the companion publication NCI **Investigational Drugs: Pharmaceutical Data.**

METHOTREXATE

NSC - 740


N
N
NH2
NMeCH2
N
N
L
HO2CCH2CH2CHNHCO
NH2
CO2H
•2H2O

Chemical Name:
L-(+)-N-[p-[[2,4-diamino-6-pteridinyl) methyl]methylamino]benzoyl]glutamic acid, dihydrate

Other Names:
Methotrexate (USAN); MTX; Amethopterine; 4-amino-10-methylfolic acid

Molecular Formula: $C_{20}H_{22}N_8O_5 \cdot 2H_2O$ **M.W.:** 490.5

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
258 ± 2 nm	22,800 - 25,200
303 ± 2 nm	23,200 - 25,200
372 ± 2 nm	7,350 - 8,200

BEST COPY AVAILABLE

High Performance Liquid Chromatography:

Column: 300 mm x 4 mm ID Spherisorb ODS

Mobile Phase: 20% CH_3OH in 0.1 M KH_2PO_4 at pH 6.7

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Sample Preparation: 1-mg sample in 1.0 ml 0.02 N NaOH or internal standard solution

Internal Standard: 5mg 4-deoxy-4-amino-N^{10}-methylpteroic acid/5 ml 0.02 N NaOH

Retention Volume: 11.5 ml (NSC-740)
19.0 ml (I.S.)

Optical Rotation:

(c = 1, 0.05 M Na_2CO_3) $[\alpha]^{20}_D = +17.0 - 19.5°$

Toxicity Data:

Man(iv): TD_{Lo}: 740 mg/kg
Archives of Internal Medicine, 136,1321,(1976)

Mouse(ip): LD_{50}: 50 mg/kg
Anatomical Record 178,465,(1974)

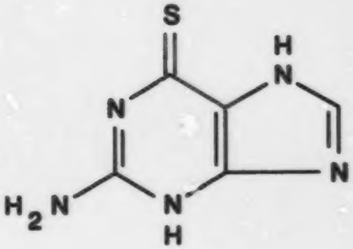
Rat(po): LD_{50}: 135 mg/kg
Drugs in Japan. Ethical Drugs, 6th Ed., (1982). p841

Rat(ip): LD_{50}: 6 mg/kg

Drugs in Japan. Ethical Drugs, 6th Ed., (1982), p841

THIOGUANINE

NSC - 752



Chemical Name:
Purine-6-thiol, 2-amino-

Other Names:
Thioguanine (USAN); 6-TG; 6-Thioguanine

Molecular Formula: $C_5H_5N_5S$ **M.W.:** 167.2

Approximate Solubility:
Readily soluble in dilute aqueous alkali. Insoluble in water, alcohol, or chloroform.

Stability:

Bulk:
The compound is stable in solid form at room temperature in the absence of moisture.

BEST COPY AVAILABLE

Solution:

Alkaline solutions slowly undergo decomposition. Alkaline solutions should not be heated above 37° C.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max}	ε
257 ± 2 nm	8,000 - 8,400
347 ± 2 nm	20,600 - 30,000

High Performance Liquid Chromatography:

Column: µBondapak C18, 300 x 4 mm ID

Mobile Phase: 3% MeOH in 0.1 M KH_2PO_4, pH = 4.5

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 2.0 mg/ml (0.1 N NaOH)

Internal Standard: thymine

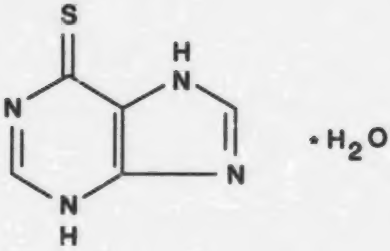
Retention Volume: 10.5 ml (NSC - 752)
15.0 ml (I.S.)

Toxicity Data:

Rat(ip): LD_{50}: 300 mg/kg
Journal of Reproduction and Fertility, 4,291,(1962)

MERCAPTOPURINE

NSC - 755



Chemical Name:
Purine-6-thiol, hydrate

Other Names:
Mercaptopurine (USAN); 6-Mercaptopurine;
Purine-6-thiol, monohydrate; 6-MP

Molecular Formula: $C_5H_4N_4S \cdot H_2O$ **M.W.:** 170.2

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 325 \pm 2$ nm $\varepsilon = 19{,}800 - 20{,}400$

BEST COPY AVAILABLE

High Performance Liquid Chromatography:

Column: 1 m x 2 mm stainless steel column packed with Vydac cation exchange packings

Solvent: 0.01 M, pH 2.25 phosphate buffer

Flow Rate: 0.9 ml/minute

Detection: UV at 254 nm

Toxicity Data:

Rat(ip): LD_{50}: 200 mg/kg
Journal of Reproduction and Fertility, 4,291,(1962)

Rat(iv): LD_{50}: 250 mg/kg
Arzneimittel-Forschung, 20,1467,(1970)

Mouse(po): LD_{50}: 280 mg/kg
Russian Pharmacology and Toxicology, 42,79,(1979)

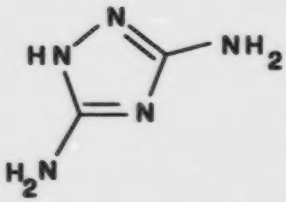
Mouse(sc): LD_{50}: 100 mg/kg
Journal of Medicinal Chemistry, 18,320,(1975)

Mouse(iv): LD_{50}: 80 mg/kg
Cancer Research, 42,122,(1982)

Mouse(ip): LD_{50}: 80 mg/kg
Cancer Research, 42,122,(1982)

GUANAZOLE

NSC - 1895



Chemical Name:
1H-1,2,4,-triazole-3,5-diamine

Other Name:
Guanazole

Molecular Formula: $C_2H_5N_5$ **M.W.:** 99.1

Approximate Solubility:	(mg/ml)
Water	200 mg/ml
Methanol	soluble
Ethanol	difficultly soluble
Ether	insoluble
Chloroform	insoluble
Benzene	insoluble

BEST COPY AVAILABLE

Stability:

Bulk:

The bulk drug stored at 60° C. for 60 days showed no decomposition. (Paper Chromatography)

Solution:

A solution (100 mg/ml in water) stored at room temperature for 24 hours showed no decomposition. (UV)

Ultraviolet Absorption:

(H_2O)

$\lambda_{max} = 208 \pm 2$ nm $\varepsilon = 6{,}180 - 6{,}480$

High Performance Liquid Chromatography:

Column: Waters Associates µBondapak C18, 300 x 3.9 mm ID

Mobile Phase: CH_3CN/water containing 0.01 M heptane sulfonic acid and sulfuric acid to adjust pH to 2.5, 10/90, v/v

Flow Rate: 1 ml/min

Detection: UV at 220 nm

Sample Preparation: 0.1 mg sample per ml water or internal standard solution.

Internal Standard: thymidine (0.5 mg/ml in water)

Retention Volume: 12.5 ml (NSC - 1895)
5.5 ml (I.S.)

Toxicity Data:

Human(iv): TD_{Lo}: 8620 mg/kg/5D
Cancer Chemotherapy Reports, 59,1117,(1975)

N-METHYLFORMAMIDE

NSC - 3051

$\mathrm{MeNHCH{=}O}$

Chemical Name:
Formamide, N-methyl-

Other Names:
N-methylformamide; NMF

Molecular Formula: C_2H_5NO **M.W.:** 59.1

Approximate Solubility:	(mg/ml)
Water	miscible
Ethanol	miscible
Ether	immiscible

Stability:

Solution:
A 25% NMF aqueous solution is stable at room temperature for at least one week (NMR).

Ultraviolet Absorption:
The spectrum shows an end absorption with a small shoulder at 280 nm.

High Performance Liquid Chromatography:

Column: 3.9 mm ID x 30 cm μBondapak C18

Mobile Phase: 3% CH_3CN in water

Flow Rate: 1 ml/min

Detection: UV at 220 nm

Sample Preparation: 8 mg/ml in mobile phase or internal standard solution

Internal Standard: dimethylacetamide (2mg/ml in mobile phase)

Retention Volume: 4.5 ml (NSC - 3051)
9.0 ml (I.S.)

Toxicity Data:

Rat(po): LD_{50}: 4000 mg/kg
Journal of Reproduction and Fertility, 4,219,(1962)

Rat(ip): LD_{50}: 3500 mg/kg
Journal of Reproduction and Fertility, 4,219,(1962)

Mouse(po): LD_{50}: 2600 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(ip): LD_{50}: 2300 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(sc): LD_{50}: 3100 mg/kg
Dissertation Abstracts International, 40,549,(1979)

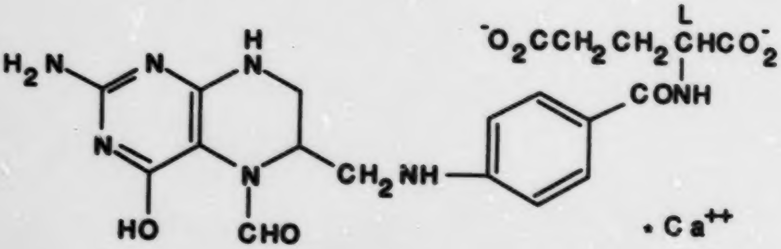
Mouse(iv): LD_{50}: 1580 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Mouse(im): LD_{50}: 2700 mg/kg
Toxicology (Elsevier), 34,173,(1985)

Dog(iv): LD10: 1262 mg/kg
National Technical Information Service, PB82-232158

CALCIUM LEUCOVORIN

NSC - 3590


H
H$_2$N
N
N
N
N
HO
CHO
CH$_2$NH
$^-$O$_2$CCH$_2$CH$_2$CHCO$_2^-$
L
CONH
• Ca^{++}

Chemical Name:
Glutamic acid, N-[p-[[(2-amino-5-formyl-5,6,7,8-tetrahydro-4-hydroxy-6-pteridinyl) methyl]-amino]benzoyl]-, calcium salt

Other Names:
Citrovorum Factor; Folinic Acid; Calcium Leucovorin

Molecular Formula: $C_{20}H_{23}N_7O_7 \cdot Ca$ M.W.: 511.5

Approximate Solubility:	(mg/ml)
DMSO	<< 1
H_2O	100
0.1 N NaOH	< 20

BEST COPY AVAILABLE

Stability:

Bulk:

Calcium leucovorin is stable in bulk form after 4 weeks storage at 60° C., as determined by HPLC.

Solution:

Leucovorin in 0.1 N NaOH (pH 13) and in deionized water (pH 6) was stable at room temperature under laboratory illumination for at least 24 hours as determined by HPLC.

Ultraviolet Absorption:

(0.1 N NaOH)

$\lambda_{max} = 282 \pm 2$ nm $\varepsilon = 23{,}000 - 26{,}500$

High Performance Liquid Chromatography:

Column: 30 cm x 4 mm ID Spherisorb ODS

Mobile Phase: 15% MeOH in 0.1 M KH_2PO_4, pH adjusted to 4.0

Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/ml in water or internal standard solution

Internal Standard: folic acid (1 mg/ml in 0.02 N NaOH)

Retention Volume: 12.0 ml (NSC - 3590)
20.2 ml (I.S.)

Optical Rotation:

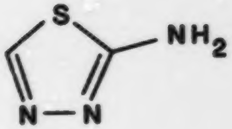
(c=1, H_2O) $[\alpha]^{21}_D = +13.0 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 732 mg/kg
Drugs in Japan. Ethical Drugs. 6,910,(1982)

2-AMINO-1,3,4-THIADIAZOLE

NSC - 4728



Chemical Name:
2-Amino-1,3,4-thiadiazole

Molecular Formula: $C_2H_3N_3S$ **M.W.:** 101.1

Approximate Solubility:	(mg/ml)
0.1 N HCl	22
4.0 N HCl	400
Water	20
Ethanol	17
Chloroform	0.35
Benzene	< 0.05
Ethyl acetate	0.8

Stability:

Bulk:

A sample stored for four weeks at 60° C. showed no decomposition by UV or TLC.

Solution:

A solution (10 mg/ml) showed no decomposition after twenty-four hours at room temperature by UV or TLC.

Ultraviolet Absorption:

(H_2O)

$\lambda_{max} = 250 \pm 2$ nm $\varepsilon = 4{,}120 - 4{,}520$

High Performance Liquid Chromatography:

Column: 50 cm x 4 mm ID Zorbax C-8

Mobile Phase: 0.1% Diethylamine in pH 6.5, 0.05 M KH_2PO_4/methanol (99/1)

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.5 mg/ml in 0.1 N HCl or internal standard solution

Internal Standard: guanosine (1 mg/ml in 0.1 N HCl)

Retention Volumes: 8.0 ml (NSC-4728)
12.5 ml (I.S.)

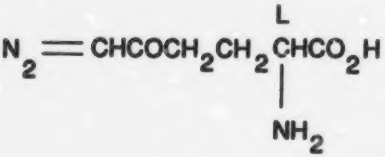
Toxicity Data:

Rat(ip): LD_{50}: 200 mg/kg
Takeda Kenkyusho Ho, 35,68,(1976)

Rat(sc): LD_{50}: 200 mg/kg
Johns Hopkins Medical Journal, 130,95,(1972)

DON

NSC - 7365



$$N_2=CHCOCH_2CH_2\underset{NH_2}{\overset{L}{C}}HCO_2H$$

Chemical Name:
Norleucine, 6-diazo-5-oxo-, L-

Other Name:
DON

Molecular Formula: $C_6H_9N_3O_3$ **M.W.:** 171.2

Approximate Solubility:
Soluble in water, insoluble in most organic solvents

Stability:

Bulk:
The compound should be stored in the deep freeze, protected from air and moisture. Material stored under these conditions shows no decomposition after 4 years.

Solution:

Solutions are unstable and should be prepared immediately before use. Solutions are most stable at pH 4.5 - 6.5.

Ultraviolet Absorption:

(pH 7.0 phosphate buffer)

$\lambda_{max} = 274 \pm 2$ nm $\varepsilon = 10{,}800 - 11{,}800$

Optical Rotation:

(c=1, H_2O) $[\alpha]^{25}_D = +14.0° \text{ to } +18.0°$

Toxicity Data:

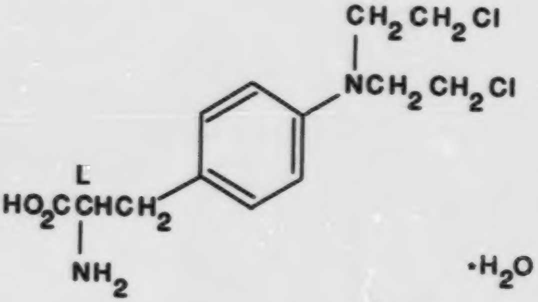
Rat(ip): LD_{50}: 80 mg/kg
Clinical Proceedings of the Children's Hospital of the District of Columbia, 18,307,(1962)

Mouse(ip): LD_{Lo}: 300 mg/kg
Journal of Endocrinology, 18,204,(1959)

Mouse(iv): LD_{50}: 74 mg/kg
Antibiotics: Origin, Nature and Properties, 2,1253,(1978)

MELPHALAN

NSC - 8806



Chemical Name:
L-Alanine, 3-(p-[bis(2-chloroethyl)amino] phenyl)-, monohydrate

Other Names:
Melphalan (USAN); L-Sarcolysin; Phenylalanine Mustard, L-PAM

Molecular Formula: $C_{13}H_{18}Cl_2N_2O_2 \cdot H_2O$ **M.W.:** 323.4

BEST COPY AVAILABLE

Approximate Solubility:	(mg/ml)
95% ethanol	< 0.9
10% aqueous ethanol	~ 1.3
Methanol	2.8 - 5.6
Water	1.7 - 2.3
Chloroform	< 1
0.1 N HCl	9 - 17
0.1 N NaOH	7 - 10.6
Acetone	< 1
pH 4 citrate buffer	2.2 - 2.6
pH 9 borate buffer	2.0 - 2.4

Stability:

Bulk:

A dried sample, stored at 60° C. for 15 days, showed about 10% decomposition as indicated by UV absorption and ionic chloride content.

Solution:

After 24 hours in water at 28° C., approximately 80% decomposition was observed as indicated by TLC.

Ultraviolet Absorption:

(H_2O)

$\lambda_{max} = 260 \pm 2$ nm $\quad\quad$ $\varepsilon = 17{,}410 - 17{,}880$

High Performance Liquid Chromatography:

Column: 300 x 3.9 mm ID, µBondapak C18

Mobile Phase: Methanol/1% acetic acid in water, 30/70, v/v

Flow Rate: 1 ml/min

Detection: UV at 254 nm

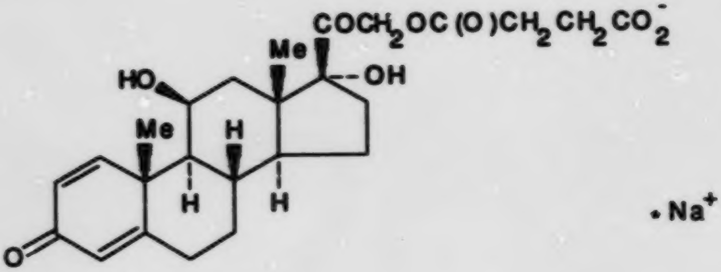
Retention Volume: 26 ml (NSC - 8806)

Optical Rotation:

(C = 0.7, methanol on a dried basis) $[\alpha]^{24}_D = -31.5 \pm 2°$

PREDNISOLONE SODIUM SUCCINATE

NSC - 9151


COCH2OC(O)CH2CH2CO2-
Me
HO
OH
Me
H
H
H
O
• Na+

Chemical Name:
Pregna-1,4-diene-3,20-dione,11β,
17,21-trihydroxy-, 21-(hydrogen succinate), sodium salt

Other Name:
Prednisolone sodium succinate

Molecular Formula: $C_{25}H_{31}O_8 \cdot Na$ **M.W.:** 482.5

Approximate Solubility:	(mg/ml)
Water	> 100
Ethanol	~ 100
Methanol	~ 100

BEST COPY AVAILABLE

Stability:

Bulk:

The compound is very hygroscopic and unstable to heat. Storage in freezer is recommended.

Ultraviolet Absorption:

(95% EtOH)

$\lambda_{max} = 242 \pm 2$ nm $\varepsilon = 14{,}300 - 15{,}300$

High Performance Liquid Chromatography:

Column: Waters Associates C18 µBondapak

Mobile Phase: Acetonitrile/water containing 1% acetic acid (30:70, v/v)

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/ml in methanol/water (30/70, v/v)

Retention Volume: 20.6 ml (NSC - 9151)

Optical Rotation:

(c = 1.1% in 95% ethanol) $[\alpha]^{25}_D = 111 \pm 3°$

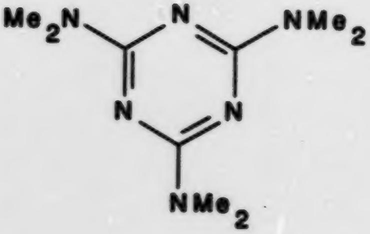
Toxicity Data:

Rat(iv): LD_{50}: 770 mg/kg
Pharmaceutical Chemistry Journal, 16,63,(1982)

Mouse(iv): LD_{50}: 1125 mg/kg
Pharmaceutical Chemistry Journal, 16,63,(1982)

HEXAMETHYLMELAMINE

NSC - 13875



Chemical Name:
s-Triazine, 2,4,6-tris(dimethylamino)-

Other Names:
HXM; Hexamethylmelamine; Altretamine

Molecular Formula: $C_9H_{18}N_6$ **M.W.:** 210.3

Approximate Solubility:	(mg/ml)
Water	0.92
Benzene	106
$CHCl_3$	220
EtOAc	52
Et_2O	47

Stability:

Bulk:
The bulk drug is stable at room temperature.

Solution:
Aqueous solutions at pH 4, 7, and 10 are stable for 24 hours at room temperature. (UV)

Ultraviolet Absorption:

(Methanol)

$\lambda_{max} = 227 \pm 2$ nm $\varepsilon = 51{,}400 - 52{,}400$

Gas-Liquid Chromatography:

Column: 10% SP-2100 on 80/120 Supelcoport; glass, 1.83 m x 2 mm ID

Carrier Gas: Helium

Flow Rate: 30 ml Helium/minute

Detection: Flame ionization

Temperatures:		
	Oven	155° C., isothermal
	Injector	250° C.
	Detector	250° C.

Internal Standard: octadecane

Retention Time: 9.6 min (NSC - 13875)
17.8 min (I.S.)

Toxicity Data:

Human(po): TD_{Lo}: 8 mg/kg
Cancer Chemotherapy Reports, 56,505,(1972)

Rat(po): LD_{50}: 350 mg/kg
Principles of Insect Chemosterilization, 315,(1968)

Rat(ip): LD_{50}: 265 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 100,398,50

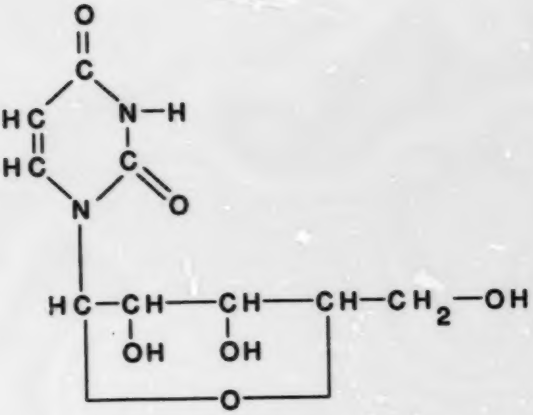
Mouse(po): LD_{50}: 437 mg/kg
Archives Internationales de Pharmacodynamie et de Therapie, 160,83,(1966)

Mouse(ip): LD_{10}: 200 mg/kg
Cancer Research, 40,2762,(1980)

Mouse(iv): LD_{50}: 171 mg/kg
National Technical Information Service, PB293-046

URIDINE

NSC - 20256



Chemical Name:
Uracil, 1-β-D-ribofuranosyl-

Molecular Formula: $C_9H_{12}N_2O_6$ **M.W.:** 244.2

Approximate Solubility:
Soluble in H_2O, and DMSO. Insoluble in ether and hexane

Ultraviolet Absorption:

(pH 7 buffer)

$\lambda_{max} = 261 \pm 2$ nm $\varepsilon = 9{,}600 - 10{,}200$

High Performance Liquid Chromatography:

Column: 4.6 mm x 25 cm ODS Spherisorb 10

Mobile Phase: 0.5 M pH 6.6 KH_2PO_4 buffer/CH_3OH, 19/1

Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

Sample Preparation: 1.3 mg/ml in mobile phase

Retention Volume: 5.7 ml (NSC - 20256)

Optical Rotation:

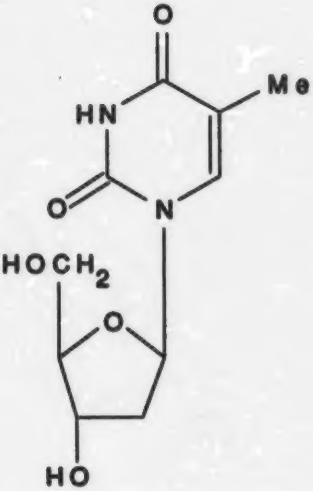
(C=2, H_2O) $[\alpha]^{20}_D = 9.4 \pm 2°$

Toxicity Data:

Mouse(ip): LD_{50}: 4335 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 207,504,(1978)

THYMIDINE

NSC - 21548



Chemical Name:
2,4(1H,3H)-pyrimidinedione, 1-(2-deoxy-β-D-ribofuranosyl)-5-methyl-

Other Name:
Thymidine

Molecular Formula: $C_{10}H_{14}N_2O_5$ **M.W.:** 242.2

Approximate Solubility:	(mg/ml)
Water	50

Stability:

Solution:

A 1% solution of thymidine in water, kept at room temperature, is stable for at least 24 hours. (HPLC)

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 267 \pm 2$ nm $\varepsilon = 9{,}700 - 9{,}900$

High Performance Liquid Chromatography:

Column: 30 cm x 4 mm ID Spherisorb ODS

Mobile Phase: 1% dioxane in 0.1 M KH_2PO_4

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg samples in 2.0 ml water
or 2.00 ml internal standard solution

Internal Standard: adenosine (0.5 mg/ml in water)

Retention Volumes: 13 ml (NSC - 21548)
21 ml (I.S.)

Optical Rotation:

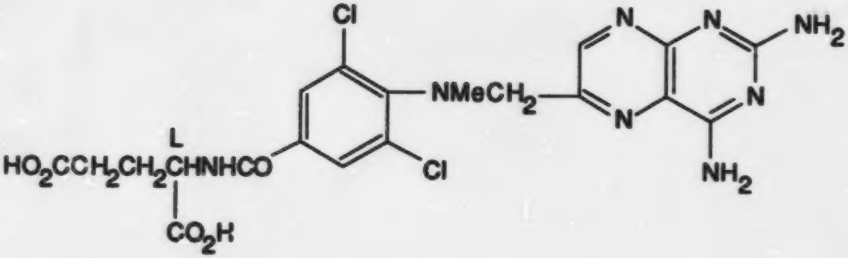
(c = 1, H_2O) $[\alpha]^{25}_D = +18.5 \pm 0.5°$

Toxicity Data:

Mouse(ip): LD_{50}: 2512 mg/kg
Journal of Pharmacology & Experimental Therapeutics, 207,504,(1978)

DICHLOROMETHOTREXATE

NSC - 29630



Cl
NMeCH2
N
N
NH2
N
N
L
HO2CCH2CH2CHNHCO
Cl
NH2
CO2H

Chemical Name:
Glutamic acid, N-[3,5-dichloro-4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-

Other Name:
Dichloromethotrexate

Molecular Formula: $C_{20}H_{20}Cl_2N_8O_5$ **M.W.:** 523.3

Approximate Solubility:	(mg/ml)
Water	< 0.05
0.1 N HCl	0.1
0.1 N NaOH	32
100% Ethanol	< 0.05
30% Ethanol	< 0.2
10% Ethanol	< 0.05

Stability:

Bulk:

A sample stored at 4° C. for 40 days showed no decomposition as indicated by paper chromatography and ultraviolet absorption. A sample stored at 60° C. for 40 days did not show any decomposition as indicated by UV absorption but the paper chromatography indicated a very slight decomposition.

Solution:

A solution of 30 mg in 1 ml 0.1 N NaOH, after 14 days at room temperature, showed only a very slight decomposition as indicated by UV absorption and paper chromatography. This decomposition was estimated to be less than 5%.

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
371 ± 2 nm	7,600 - 7,780
257 ± 2 nm	25,600 - 26,200

High Performance Liquid Chromatography:

Column: Alltech Spherisorb S5 ODS, 25 cm x 4.6 mm ID

Mobile Phase: 25% MeOH in pH 6.7 0.1 M KH_2PO_4

Flow Rate: 3 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/ml in 0.02 N NaOH and diluted with an equal volume of internal standard solution

Internal Standard: o-nitroaniline (0.5 mg/ml in methanol)

Retention Volumes: 34.5 ml (NSC-29630)
17.5 ml (I.S.)

Optical Rotation:

(c = 1, 0.05 M Na_2C0_3) $[\alpha]^{21}_D = +17.1 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 1021 mg/kg
National Technical Information Service, PB82-172644

MITOGUAZONE DIHYDROCHLORIDE

NSC - 32946

$HN{=}C(NH_2)NHN{=}CHCMe{=}NNHC(NH_2){=}NH$

$\cdot 2HCl \cdot H_2O$

Chemical Name:
Guanidine, 1,1'-[(methylethanediylidene) dinitrilo]di-,dihydrochloride, monohydrate

Other Names:
Methylglyoxal Bisguanylhydrazone Dihydrochloride Monohydrate; Methyl GAG; Methyl-G; Mitoguazone Dihydrochloride

Molecular Formula: $C_5H_{12}N_8 \cdot 2HCl \cdot H_2O$ **M.W.:** 275.1

Approximate Solubility:	(mg/ml)
0.1 N NaOH	soluble
Water	> 100
0.01 N NaOH	partly soluble
0.1 N HCl	partly soluble
MeOH	partly soluble
50% EtOH	partly soluble

Stability:

Solution:

A solution of 100 mg/ml in water stored at room temperature for 44 days showed no decomposition.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 283 ± 2 nm ϵ = 36,200 - 40,000

High Performance Liquid Chromatography:

Column: 4 mm ID x 300 mm Spherisorb ODS

Mobile Phase: 4% acetonitrile in 0.1 M KH_2PO_4, pH adjusted to 3.8

Flow Rate: 2 ml/min

Detection: UV at 210 nm

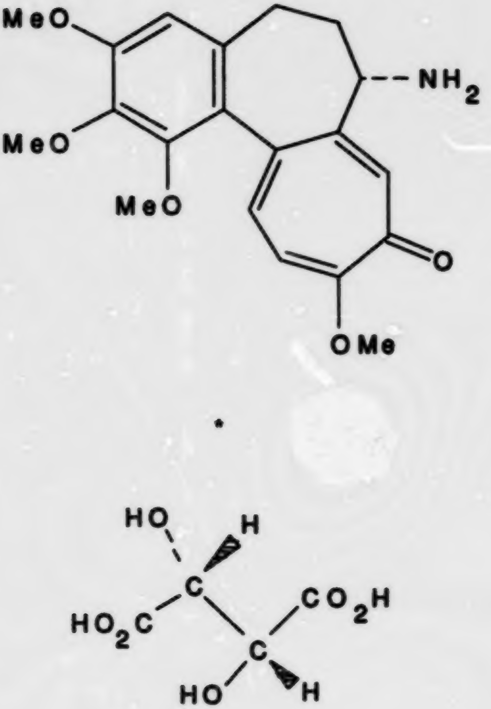
Sample Preparation: 1 mg/ml in water or internal standard solution

Internal Standard: 1-naphthol-4-sulfonic acid Na salt (7 mg in 25ml water)

Retention Volumes: 8.0 ml (NSC-32946)
11.0 ml (I.S.)

TMCA

NSC - 36354


MeO
MeO
MeO
NH2
O
OMe
•
HO
H
C
HO2C
CO2H
C
HO
H

Chemical Name:
Benzo[a]heptalen-9(5H)-one, 7-amino-6,7-dihydro-1,2,3,10-tetramethoxy-,[R-(R*,R*)]-2,3-dihydroxy-butanedioate (1:1)

Other Names:
TMCA; Trimethylcolchicinic acid, methyl ester, L-tartrate (1:1)

BEST COPY AVAILABLE

Molecular Formula: $C_{20}H_{23}NO_5{\cdot}C_4H_6O_6$ **M.W.:** 507.5

Approximate Solubility: (mg/ml)

Water	15
Ethanol	1

Ultraviolet Absorption:

(pH 7 phosphate buffer)

$\lambda_{max} = 243 \pm 2$ nm $\varepsilon = 34{,}200 - 34{,}800$

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18,
300 x 3.9 mm

Mobile Phase: Methanol/0.01 M pH 7 phosphate buffer
55/45, v/v

Flow Rate: 1 ml/min

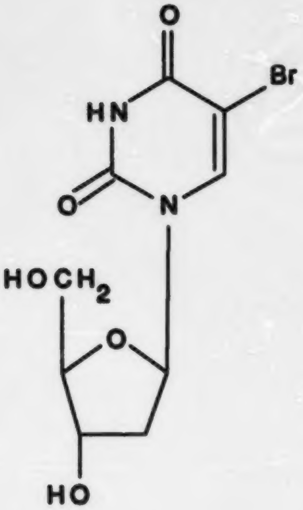
Detection: UV at 254 nm

Sample Preparation: Sample concentration approximately
0.2 mg/ml in mobile phase.

Retention Volume: 8.5 ml (NSC - 36354)

BROMODEOXYURIDINE

NSC - 38297



Chemical Name:
Uridine, 5-bromo-2'-deoxy-

Other Names:
Bromodeoxyuridine; BUdR

Molecular Formula: $C_9H_{11}N_2O_5Br$ **M.W.:** 307.1

Approximate Solubility: (mg/ml)

Water	10 - 20
Dimethylacetamide	~ 200
1 N NaOH	> 400
Dimethylsulfoxide	~ 160
Acetone	~ 4

Stability:

Bulk:

The bulk drug should be stored in tightly closed containers at controlled room temperature.

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 280 \pm 2$ nm $\varepsilon = 8,900 - 9,400$

High Performance Liquid Chromatography:

Column: 30 cm x 3.2 mm Spherisorb ODS

Mobile Phase: 6% MeOH/0.1 M phosphate buffer, pH 5.5

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/2 ml in water or internal standard solution

Internal Standard: benzoic acid (0.8 mg/ml in water)

Retention Volumes: 15.0 ml (NSC-38297)
7.0 ml (I.S.)

Optical Rotation:

(C = 1, 0.1 N NaOH) $[\alpha]^{20}_D = +31 \pm 1°$

Toxicity Data:

Rat(po): LD_{50}: 8400 mg/kg
Iyakuhin Kenkyu, 4,467,(1973)

Rat(ip): LD_{50}: 1500 mg/kg
Advances in Teratology, 3,181,(1968)

Rat(sc): LD_{50}: 3900 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Rat(iv): LD_{50}: 2320 mg/kg
Takeda Kenkyusho Ho, 30,735,(1971)

Mouse(po): LD_{50}: 9100 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

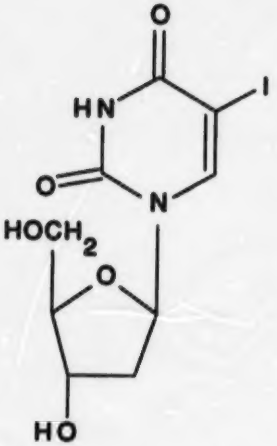
Mouse(ip): LD_{50}: 3050 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Mouse(sc): LD_{50}: 3500 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

Mouse(iv): LD_{50}: 2500 mg/kg
Takeda Kenkyusho Ho, 30,530,(1971)

IODODEOXYURIDINE

NSC - 39661



Chemical Name:
Uridine, 2'-deoxy-5-iodo-

Other Names:
Idoxuridine (USAN); 5-IUdR

Molecular Formula: $C_9H_{11}IN_2O_5$ **M.W.:** 354.1

Approximate Solubility:	(mg/ml)
0.1 N NaOH	30
0.1 N HCl	2
H_2O	2

Stability:

Solution:

An aqueous solution (2 mg/ml) shows no decomposition after 24 hours at room temperature. (UV and paper chromatography)

Ultraviolet Absorption:

(Water)

$\lambda_{max} = 288 \pm 2$ nm $\varepsilon = 7{,}500 - 7{,}800$

High Performance Liquid Chromatography:

Column: 4.6 mm ID x 25 cm Alltech Spherisorb S5 ODS

Mobile Phase: 2% CH_3CN in water

Flow Rate: 2.5 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/ml in water or internal standard solution

Internal Standard: adenosine (0.3 mg/ml in 0.01 N NaOH)

Retention Volumes: 31 ml (NSC - 39661)
36 ml (I.S.)

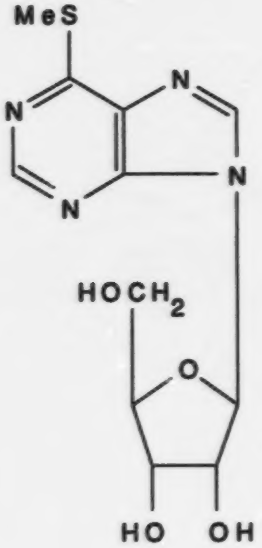
Toxicity Data:

Rat(ip): LD_{50}: 4000 mg/kg
Advances in Teratology, 3,181,(1968)

Mouse(ip): LD_{50}: 1000 mg/kg
Journal of the National Cancer Institute, 62,911,(1979)

6-METHYLMERCAPTOPURINE RIBOSIDE

NSC - 40774



Chemical Name:
9H-Purine, 6-methylthio-9-β-D-ribofuranosyl-

Other Names:
6-MMPR; 6-Methyl MP-riboside; 6-Methylmercaptopurine riboside

Molecular Formula: $C_{11}H_{14}N_4O_4S$ **M.W.:** 298.3

Approximate Solubility:

	(mg/ml)
DMA	167
50% DMF	50
H_2O	25
Propylene glycol	6

Stability:

Bulk:

The compound is stable to light and air, mildly decomposed by heat and acid, and is totally degraded by base and peroxidant. (HPLC)

Solution:

A saturated solution at room temperature showed no detectable decomposition after 10 days as indicated by paper chromatography.

Ultraviolet Absorption:

(Water)

λ_{max}	ε
292 ± 2 nm	19,000 - 19,600
224 ± 2 nm	11,500 - 12,200

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18,
300 mm x 3.9 mm ID

Mobile Phase: Acetonitrile/water, 12/88, v/v

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.2 mg/ml in water or internal standard solution

Internal Standard: acetanilide (0.05 mg/ml in water)

Retention Volumes: 13 ml (NSC - 40774)
20 ml (I.S.)

Optical Rotation:

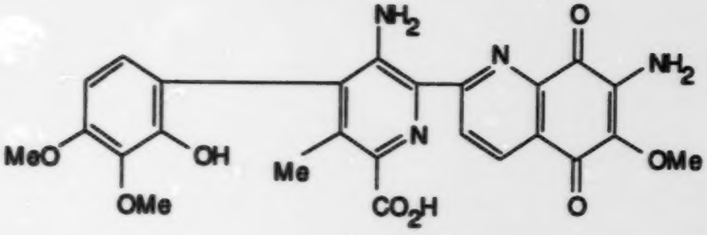
(c = 1, H_2O) $[\alpha]^{22}_D = -58.0 \pm 2°$

Toxicity Data:

Rat(ip): LD_{50}: 65 mg/kg
Archives of Pathology, 86,395,(1968)

STREPTONIGRIN

NSC - 45383



Chemical Name:
Picolinic acid, 5-amino-6-(7-amino-5,8-dihydro-6-methoxy-5,8-dioxo-2-quinolyl)-4-(2-hydroxy-3,4-dimethoxyphenyl)-3-methyl-

Other Names:
Streptonigrin (USAN); BA-163; PC-501

Molecular Formula: $C_{25}H_{22}N_4O_8$ **M.W.:** 506.5

Approximate Solubility:
Soluble in tetrahydrofuran or dioxane

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
379 ± 2 nm	16,680 - 18,800
246 ± 2 nm	39,050 - 44,100

High Performance Liquid Chromatography:

Column: 300 x 3.9 mm ID, μBondapak C18

Mobile Phase: Methanol/0.01 M phosphate buffer, pH 7, 35/65, v/v

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.02 mg/ml in mobile phase or internal standard solution

Internal Standard: propriophenone (14 μl/liter in mobile phase)

Retention Volumes: 6.5 ml (NSC - 45383)
14 ml (I.S.)

Toxicity Data:

Mouse(po): LD_{50}: 2330 μg/kg
Antibiotiki, 12,132,(1967)

Mouse(ip): LD_{50}: 750 µg/kg
CRC Handbook of Antibiotic Compounds, 3,332,(1980)

Mouse(sc): LD_{50}: 1000 µg/kg
Comptes Rendus Hebdomadaires des Seances, 261,4911,(1965)

Mouse(iv): LD_{50}: 500 µg/kg
Antibiotics: Origin, Nature and Properties, 2,1359,(1978)

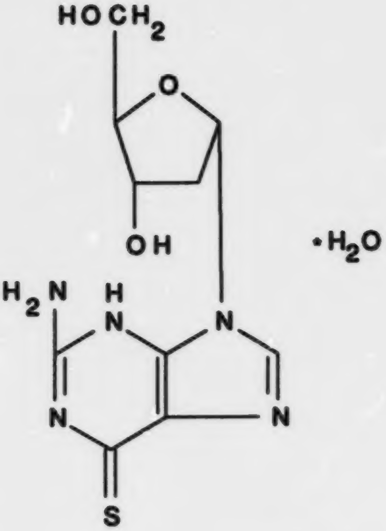
Dog(po): LD_{50}: 500 µg/kg
Antibiotiki, 11,1090,(1966)

Rabbit(po): LD_{50}: 570 mg/kg
Japanese Journal of Antibiotics, 29,439,(1976)

Rat(iv): LD_{50}: 600 µg/kg
Antibiotiki, 12,132,(1967)

ALPHA-TGdR

NSC - 71851



Chemical Name:
9H-Purine-6-thiol, 2-amino-9-(2-deoxy-
α-D-erythro-pentofuranosyl)- monohydrate

Other Names:
Alpha-2'-Deoxythioguanosine Hydrate;
Alpha-TGdR

Molecular Formula: $C_{10}H_{13}N_5O_3S \cdot H_2O$ **M.W.:** 301.3

Approximate Solubility:

Solvent	(mg/ml)
Water	7.1
DMSO	18
DMA	22
0.1 N NaOH	4.6
Chloroform	< 0.3
95% Ethanol	2.0
Propylene glycol	3.0

Stability:

Bulk:
A sample stored at 60° C. for 28 days showed no decomposition as determined by UV and TLC.

Solution:
Dilute solutions in H_2O (6 mg/ml) are stable for approximately 24-48 hours at room temperature as determined by UV and TLC.

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
252 ± 2 nm	13,300 - 14,500
317 ± 2 nm	19,500 - 21,200

High Performance Liquid Chromatography:

Column: Waters RCM, C-18 cartridge

Mobile Phase: 5% acetonitrile in 0.05 M KH_2PO_4
pH = 4.5

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 1.5 mg/2.0 ml water or internal standard solution

Internal Standard: inosine (0.3 mg/ml in water)

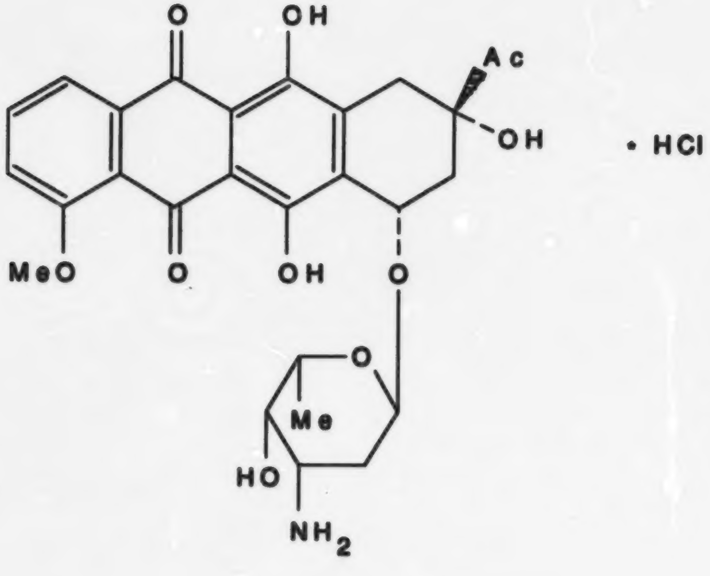
Retention Volumes: 14.0 ml (NSC - 71851)
8.0 ml (I.S.)

Optical Rotation:

(c=1, 0.1 N NaOH) $[\alpha]^{21}_D = +78 \pm 2°$

DAUNORUBICIN HYDROCHLORIDE

NSC - 82151



Chemical Name:

L-lyxo-Hexopyranoside, 3β-acetyl-1,2,3,4,6,11-hexahydro-3,5,12-trihydroxy-10-methoxy-6,11-dioxo-1α-naphthacenyl-3-amino-2,3,6-trideoxy-, α-, hydrochloride

Other Names:

Daunorubicin Hydrochloride (USAN); Daunomycin Hydrochloride; Rubidomycin Hydrochloride

Molecular Formula: $C_{27}H_{29}NO_{10}\cdot HCl$ **M.W.:** 564.0

Approximate Solubility:

Solubility in water > 450 mg/ml (by UV). At this concentration the solution is dark red and viscous.

Stability:

Bulk:

Crystalline drug which has been stored for two years at room temperature in the dark shows no decomposition as determined by spectroscopic, chromatographic, or optical rotation methods.

Solution:

In the dark, aqueous solutions (C = 0.02% of daunomycin hydrochloride) are stable for 24 hours at room temperature.

Ultraviolet Absorption:

(pH 7.0 buffer)

λ_{max}	$\varepsilon^1{}_1$
233 ± 2 nm	590 - 690
253 ± 2 nm	385 - 480
290 ± 2 nm	130 - 150
482 ± 2 nm	185 - 195
495 ± 2 nm	180 - 195

High Performance Liquid Chromatography:

Column: 30 cm x 4 mm ID Lichrosorb RP8

Mobile Phase: CH_3OH/0.1 M KH_2PO_4, pH 6.7, 1/1

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/2 ml water or internal
standard solution

Internal Standard: doxorubicin hydrochloride
(0.8 mg/2 ml)

Retention Volumes: 24 ml (NSC - 82151)
12 ml (I.S.)

Toxicity Data:

Rat(po): LD_{50}: 290 mg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Rat(ip): LD_{50}: 14300 µg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Rat(sc): LD_{50}: 33200 µg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Rat(iv): LD_{50}: 14300 µg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Mouse(po): LD_{50}: 205 mg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

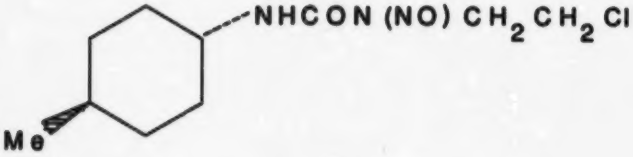
Mouse(ip): LD_{50}: 3050 μg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Mouse(sc): LD_{50}: 28800 μg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

Mouse(iv): LD_{50}: 16700 μg/kg
Drugs in Japan. Ethical Drugs, 6,437,(1982)

SEMUSTINE

NSC - 95441



Chemical Name:
Urea, 1-(2-chloroethyl)-3-(4-methylcyclohexyl)-1-nitroso-

Other Names:
Methyl CCNU; Semustine (USAN)

Molecular Formula: $C_{10}H_{18}ClN_3O_2$ **M.W.:** 247.7

Approximate Solubility:	(mg/ml)
Water	0.09
0.1 N HCl	0.09
0.1 N NaOH	0.09
10% Ethanol	0.1
Absolute ethanol	100
DMSO	250
Chloroform	667

BEST COPY AVAILABLE

Stability:

Bulk:
A sample stored at room temperature for 30 days showed 4% decomposition. (UV)

Solution:
A refrigerated solution in 10% EtOH decomposed 2% in 6 hours while a solution at room temperature showed 25% decomposition in 6 hrs. (UV) Solutions in methanol were also found to be unstable by UV analysis.

Ultraviolet Absorption:

(MeOH)

$\lambda_{max} = 229 \pm 2$ nm $\varepsilon = 6{,}000 - 6{,}190$

High Performance Liquid Chromatography:

Column: Waters μBondapak C18, 300 x 3.9 mm ID

Mobile Phase: CH_3CN/1% HOAc (aq), 70/30, v/v

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

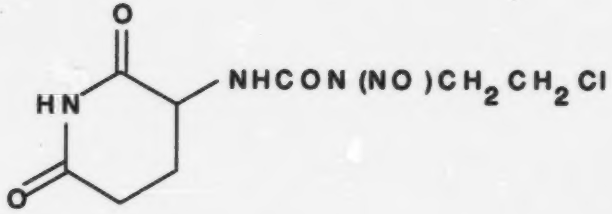
Sample Preparation: Weighed amounts of the test sample (approximately 20 mg) in 10 ml flasks are dissolved in internal standard solution. These solutions are diluted 3 to 25 ml to give a concentration of 0.25 mg/ml.

Internal Standard: fluoranthrene (0.08 mg/ml in acetonitrile)

Retention Volume: 5.5 ml (NSC - 95441)
9.0 ml (I.S.)

PCNU

NSC - 95466



Chemical Name:
Urea, 1-(2-chloroethyl)-3-(2,6-dioxo-3-piperidyl)-1-nitroso-

Other Name:
PCNU

Molecular Formula: $C_8H_{11}ClN_4O_4$ **M.W.:** 262.7

Approximate Solubility:	(mg/ml)
Water	< 1
Water pH 4	< 1
Water pH 9	2-3
10% EtOH	< 1
95% EtOH	2 - 3
MeOH	3 - 4
$CHCl_3$	1 - 3
Acetone	12.5 - 15

Stability:

Bulk:

A sample stored at 60° C. for 10 days decomposed 18% (UV). The compound was found to be stable in bulk form at room temperature exposed to lab light through 60 days, as monitored by UV, TLC and ionic chloride determinations.
For long-term storage the bulk compound should be protected from moisture and stored at -15° C.

Solution:

The compound dissolved in 3% methanol/ water decomposed 4% in one hour, 6.5 % in three hours 15% in six hours and 38% in 24 hours as indicated by UV. There was no formation of ionic chloride during the 24 hours. Solutions should be prepared immediately before use.

High Performance Liquid Chromatography:

Column: Waters µBondapak C18, 300 x 3.9 mm ID

Mobile Phase: CH_3CN/1% HOAc (aq.), 15/85, v/v

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.45 mg/ml in internal standard solution.

Internal Standard: Acetonitrile containing 0.04 µl acetophenone per ml as the internal standard/1% HOAC (aq), 50/50, (v/v).

Retention Volume: 11.0 ml (NSC - 95466)
23.0 ml (I.S.)

Ultraviolet Absorption:

(3% Methanol/water)

$\lambda_{max} = 230 \pm 2$ nm ε = 6,052 - 6,270

Toxicity Data:

Mouse(po): LD_{50}: 35700 µg/kg
National Technical Information Service, PB282-250

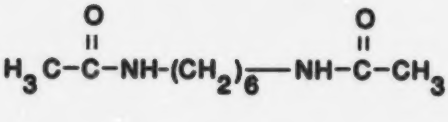
Mouse(iv): LD_{50}: 22 mg/kg
National Technical Information Service, PB282-250

Dog(iv): LD_{Lo}: 3 mg/kg
National Technical Information Service, PB282-250

Monkey(iv): LD_{Lo}: 10 mg/kg
National Technical Information Service, PB282-250

HMBA

NSC - 95580



$H_3C-\overset{\overset{O}{\|}}{C}-NH-(CH_2)_6-NH-\overset{\overset{O}{\|}}{C}-CH_3$

Chemical Name:
Acetamide, N,N'-hexamethylenebis-

Other Name:
HMBA

Molecular Formula: $C_{10}H_{20}N_2O_2$ **M.W.:** 200.3

Approximate Solubility:	(mg/ml)
H_2O	> 50
pH 4 Acetate buffer	> 50
pH 9 Carbonate buffer	> 50
0.1 N NaOH	> 50
0.1 N HCl	> 50
10% Ethanol	> 50
95% Ethanol	> 50
Methanol	> 50

Stability:

Bulk:

A sample stored at 60° C. in the dark for 30 days retained 99 ± 2% of its potency. (GC)

Solution:

Samples were dissolved in water at a concentration of 20 mg/ml and stored in clear glass containers at room temperatures under normal laboratory light for 9 days. The sample retained 98 ± 2% of its potency. (GC)

Gas Chromatography:

Column: Packed glass, 10% OV-17 on Gas Chrom Q, 100/120 Mesh, 1.83 m x 2 mm I.D.

Carrier Gas: Helium

Flow Rate: 30 ml/min

Detection: FID

Temperatures:		
	Oven	205° C.
	Injector	250° C.
	Detector	250° C.

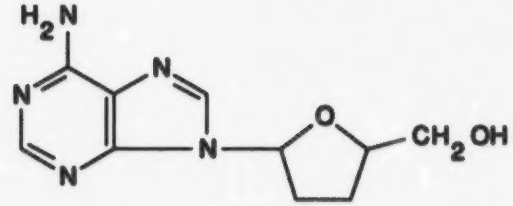
Sample Preparation: 1 mg/ml in internal standard solution

Internal Standard: pentacosane (0.6 mg/ml in isopropanol/hexane, 70/30)

Retention Times: 6.4 min (NSC - 95580)
10.3 min (I.S.)

DIDEOXYADENOSINE

NSC-98700



Chemical Name:
2',3'-dideoxyadenosine

Other Name:
Dideoxyadenosine; DDA

Molecular Formula: $C_{10}H_{13}N_5O_2$ **M.W.:** 235.2

Approximate Solubility: (mg/ml)

H_2O	3.4-5.1
Buffer, pH4	4.8-9.6
Buffer, pH9	3.2-4.8
EtOH	1.6-2.0
DMA	2.6-3.4
DMSO	3.3-5.0
$CHCl_3$	< 0.7
EtOAc	< 0.7
t-BuOH	< 0.7

Stability:

Bulk:
2',3'-Dideoxyadenosine is stable as a bulk chemical for at least 6 weeks at room temperature and 45° C., under light or dark conditions.

Solution:
DDA is stable as a 0.1 mg/ml water solution for at least 23 hrs at room temperature.

Ultraviolet Absorption:

λ_{max}	ε
260 ± 2nm	14,500 ± 500
208 ± 2nm	19,500 ± 700

High Performance Liquid Chromatography:

Column : IBM C8, 250 x 4.5 mm I.D.

Mobile Phase: 8% CH_3CN in 0.05M $NH_4H_2PO_4$ (pH unadjusted)

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/10 ml of internal standard solution. Sonicate samples 10 minutes before injection.

Internal Standard: Approx. 4 mg orcinol/ml in MeOH/H_2O (50:50).

Retention Volumes: 9.5 ml (NSC 98700)
18.3 ml (I.S.)

Optical Rotation:

($C = 1$, H_2O) $[\alpha]^{25}_D = -28 \pm 2°$

Toxicity Data:

Mouse(po): LD_{50}: 5 gm/kg
Antimicrobial Agents & Chemotherapy, 19,424,(1981)

Mouse(sc): LD_{50}: 1320 mg/kg
Antimicrobial Agents & Chemotherapy, 19,424,(1981)

YOSHI-864

NSC - 102627

$MeSO_2O(CH_2)_3NH(CH_2)_3OSO_2Me$

$\cdot HCl$

Chemical Name:
1-Propanol, 3,3'-iminodi-, dimethanesulfonate (ester), hydrochloride

Other Name:
Yoshi-864

Molecular Formula: $C_8H_{19}NO_6S_2 \cdot HCl$ **M.W.:** 325.8

Approximate Solubility:	(mg/ml)
Water	> 300
Dimethylsulfoxide	40
Ethanol	Very slightly soluble
Methanol	Very slightly soluble
Ether	Insoluble
Benzene	Insoluble
Chloroform	Insoluble
Ethyl acetate	Insoluble
Acetonitrile	Insoluble

Stability:

Bulk:

Bulk samples are stable at room temperature for 4 weeks (NMR). It is necessary to store the compound in a refrigerator or in a cold room.

Solution:

Yoshi-864 should be stable in H_2O at room temperature for up to 1 hour and in H_2O at 0° C. for 24 hours (provided the rate of decomposition in D_2O and H_2O are comparable). (NMR)

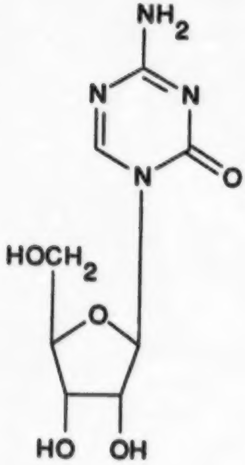
Toxicity Data:

Rat(iv): LD_{50}: 75 mg/kg
Arzneimittel-Forschung, 24,1139,(1974)

Mouse(ip): LD_{10}: 170 mg/kg
Journal of Medicinal Chemistry, 20,515,(1977)

AZACITIDINE

NSC - 102816


NH2
N
N
N
O
HOCH2
O
HO
OH

Chemical Name:
s-Triazin-2(1H)-one, 4-amino-1-β-D-ribofuranosyl-

Other Names:
Azacitidine (USAN); 5-Azacytidine; Ladakamycin

Molecular Formula: $C_8H_{12}N_4O_5$ **M.W.:** 244.2

Approximate Solubility:	(mg/ml)
DMSO	52.7
Distilled H_2O	13.7 - 14.0
0.1 N HCl	27.7 - 28.0
0.1 N NaOH	42.0 - 43.8
35% Ethyl alcohol	14.2 - 15.0

Stability:

Bulk:
Samples of 5-azacytidine and 5-azacytidine hydrate were found to be stable at 25° C. and 60° C. for at least 30 days.

Solution:
Dilute aqueous solutions of 5-azacytidine have been found to be unstable at 24-26° C. A 1% aqueous solution at 5-6° C. decomposes 2, 5, and 9% in 2, 8, and 24 hours respectively. At room temperature a 1% aqueous solution shows 7, 20 and 41% decomposition in 2, 8, and 24 hours respectively. (UV and NMR)

Ultraviolet Absorption:

(0.1 M acetate buffer, pH 5)

$\lambda_{max} = 242 \pm 2$ nm $\varepsilon =$ 6,850 - 7,250

High Performance Liquid Chromatography:

Column: 300 mm x 4.6 mm ID Alltech C-8

Mobile Phase: pH 6.5, 0.02 M KH_2PO_4

Flow Rate: 1.5 ml/min

Detection: UV at 210 nm

Sample Preparation: 0.5 mg of the sample is quickly dissolved in 1.0 ml of the mobile phase or internal standard solution

Internal Standard: uridine (1.5 mg/ml in mobile phase)

Retention Volumes: 6.8 ml (NSC - 102816)
9.0 ml (I.S.)

Optical Rotation:

(c = 1, H_2O) $[\alpha]^{22}_D = 40.0 \pm 1.0°$

Toxicity Data:

Woman(iv): TD_{Lo}: 500 µg/kg
Cancer Chemotherapy Reports, 56,413,(1972)

Mouse(po): LD_{50}: 572 mg/kg
Toxicology and Applied Pharmacology, 19,382,(1971)

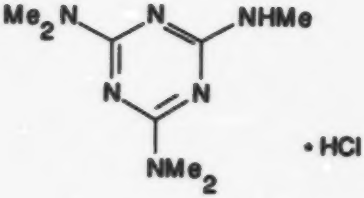
Mouse(ip): LD_{50}: 68 mg/kg
Experientia, 22,53,(1966)

Mouse(iv): LD_{50}: 229 mg/kg
National Technical Information Service, PB84-211432

Dog(iv): LD_{50}: 7200 µg/kg
Advances in Pharmacology and Chemotherapy, 14,285,(1977)

PENTAMETHYLMELAMINE HYDROCHLORIDE

NSC - 118742



Chemical Name:
Melamine, N^2,N^2,N^4,N^4,N^6-pentamethyl-, monohydrochloride

Other Name:
Pentamethylmelamine hydrochloride

Molecular Formula: $C_8H_{16}N_6 \cdot HCl$ **M.W.:** 232.7

Approximate Solubility: (as free base)

Solvent	Heat	Solubility(mg/ml)
0.1 N HCl	none; moderate	~ 15 - 20
H_2O	strong	~ 3.6
MeOH	moderate	> 150
95% EtOH	moderate	> 200
$CHCl_3$	none	> 200
DMSO	none	> 100

Stability:

Bulk:
A sample stored at 60° C. for 30 days showed no decomposition as indicated by TLC.

Solution:
A 2% solution in water (pH = 2.9), showed no decomposition after 7 days at room temperature as indicated by TLC.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 237 ± 2 nm ε = 26,200 - 27,100

High Performance Liquid Chromatography:

Column: 30 cm x 4.0 mm ID Spherisorb ODS

Mobile Phase: MeOH/H_2O/Et_2NH, 600/400/0.5

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

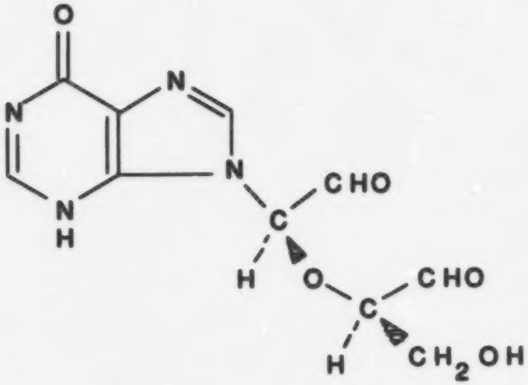
Sample Preparation: 1-mg samplings are accurately weighed and each dissolved in 1.00 ml H_20. One ml of internal standard solution is added and aliquots (1.5 µl) of the resulting solutions are injected.

Internal Standard: o-nitroaniline (2.4 mg/10 ml methanol)

Retention Volumes: 6.5 ml (NSC - 118742)
4.5 ml (I.S.)

DIGLYCOALDEHYDE

NSC - 118994



Chemical Name:
Diglycolaldehyde,α-(hydroxymethyl)-α'-(6-hydroxy-9H-purin-9-yl)-

Other Names:
Inosine Dialdehyde; Inox; Wyeth WY-5321; Diglycoaldehyde

Molecular Formula: $C_{10}H_{10}N_4O_5$ **M.W.:** 266.2

Approximate Solubility:	(mg/ml)
H_2O	500
DMSO	335
Ethanol	50
Chloroform	0.01
Ether	< 0.02
Ethyl acetate	< 0.02

BEST COPY AVAILABLE

Stability:

Bulk:

There is no detectable decomposition over a four week storage period at room temperature. Approximately 2.3% decomposition occurs at 60° C. over the same period when analyzed by HPLC, TLC and paper chromatography.

Solution:

Solutions in water, 0.04 mg/ml and 100 mg/ml acetate free inosine dialdehyde studied by UV and TLC were found to be stable at room temperature for at least 24 hours.

Ultraviolet Absorption:

(pH 7 buffer)

$\lambda_{max} = 247 \pm 2$ nm $\varepsilon = 10{,}700 - 11{,}300$

High Performance Liquid Chromatography:

Column: 2 m x 2 mm OD Reverse Phase Phenyl

Mobile Phase: Deionized water

Flow Rate: 0.4 ml/min

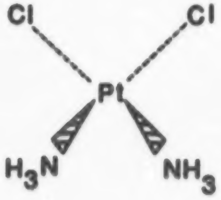
Detection: UV at 254 nm

Toxicity Data:

Mouse(iv): LD_{50}: 567 mg/kg
National Technical Information Service, PB82-166125

CISPLATIN

NSC - 119875



Chemical Name:
Platinum, diamminedichloro-, cis-

Other Names:
cis-Diamminedichloroplatinum (II); CPD; DDP;
Cisplatin (USAN)

Molecular Formula: $PtCl_2H_6N_2$ **M.W.:** 300.1

Approximate Solubility:	(mg/ml)
H_2O	1
DMSO	10
10:1 PVP coprecipitate in 10% PVP	2.5
Dimethylformamide (pure anhydrous)	24

BEST COPY AVAILABLE

Stability:

Solution:

Aqueous solutions decompose in two steps to a compound that has two water molecules replacing the two chlorine atoms. At 30° C. the half life is five hours at neutral pH.
The platinum compound is attacked by a variety of nucleophiles (i.e. hydroxide ion, pyridine, nitrate ion) which replace the chlorine atoms.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max} = 301 ± 2 nm ε = 124 - 145

High Performance Liquid Chromatography:

Column: 250 mm x 4 mm ID Zorbax NH_2

Mobile Phase: 5% H_2O in absolute EtOH

Flow Rate: 2.5 ml/min

Detection: UV at 210 nm

Sample Preparation: 1 mg/ml in 0.1 N HCl or internal standard solution

Internal Standard: guanosine (0.6 mg/ml in 0.1 N HCl)

Retention Volumes: 30 ml (NSC - 119875)
17.5 ml (I.S.)

Toxicity Data:

Human(iv): TD_{Lo}: 2500 µg/kg
Cancer Chemotherapy Reports, 59,647,(1975)

Rat(po): LD_{50}: 25800 µg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Rat(ip): LD_{50}: 8300 µg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Rat(sc): LD_{50}: 8100 µg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Rat(iv): LD_{50}: 8 mg/kg
Journal of the National Cancer Institute, 67,201,(1981)

Rat(im): LD_{50}: 9200 µg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Mouse(po): LD_{50}: 32700 µg/kg
Kiso to Rinsho. Clinical Report, 15,5669,(1981)

Mouse(ip): LD_{50}: 17400 µg/kg
Kiso to Rinsho. Clinical Report,15,5669,(1981)

Mouse(sc): LD_{50}: 16900 µg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Mouse(iv): LD_{50}: 12 mg/kg
Toxicology and Applied Pharmacology, 25,230,(1973)

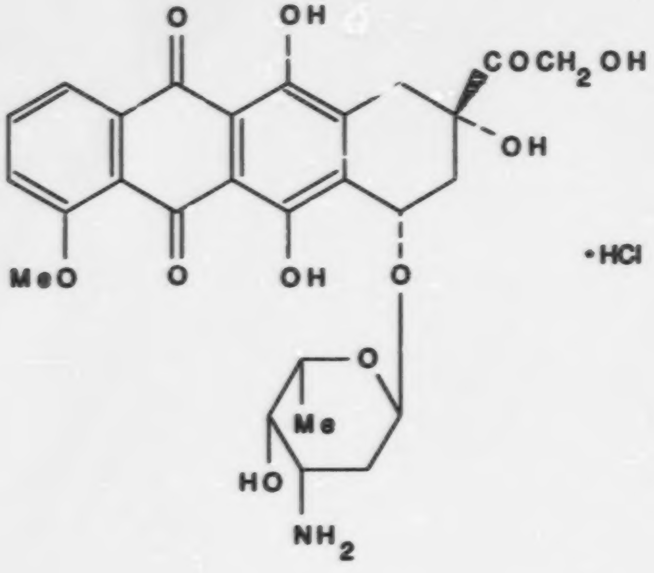
Mouse(im): LD_{50}: 17900 µg/kg
Yakuri to Chiryo. Pharmacology and Therapeutics, 10,723,(1982)

Dog(iv): LD_{Lo}: 2500 µg/kg
Toxicology and Applied Pharmacology, 25,230,(1973)

Monkey(iv): LD_{Lo}: 250 µg/kg
Cancer, 33,1219,(1974)

DOXORUBICIN HYDROCHLORIDE

NSC - 123127


O
OH
COCH2OH
OH
MeO
O
OH
O
• HCl
O
Me
HO
NH2

Chemical Name:

5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S-cis)-

Other Names:

Adriamycin hydrochloride; Doxorubicin hydrochloride (USAN)

Molecular Formula: $C_{27}H_{29}NO_{11}\cdot HCl$ **M.W.:** 579.9

Approximate Solubility:

Soluble in water, methanol and aqueous alcohol

Stability:

Bulk:

The compound should be stored in a refrigerator protected from moisture and light.

Solution:

TLC data indicate that solutions stored at room temperature, 4° C., and protected from light are stable for at least 7 days. However, a solution of doxorubicin HCl stored at room temperature and exposed to laboratory illumination showed measurable decomposition. The rate of decomposition is approximately 0.5% per day and at the end of the 7th day, 3-4% decomposition has occurred. (TLC)

Ultraviolet and Visible Absorption:

(0.1 M pH 6 phosphate buffer)

λ_{max}	ε
233 ± 2 nm	38,500 - 39,000
252 ± 2 nm	25,300 - 25,800
288 ± 2 nm	8,870 - 9,300
478 ± 2 nm	12,300 - 12,400
494 ± 2 nm	12,200 - 12,300
530 ± 2 nm	6,500 - 6,630

High Performance Liquid Chromatography:

Column: Lichrosorb RP 8, 300 mm x 4 mm ID

Mobile Phase: 0.1 M KH_2PO_4 pH 6.7/CH_3OH, 45/55

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.5 mg/ml in water or internal standard solution

Internal Standard: daunorubicin HCl (0.8 mg/ml in water)

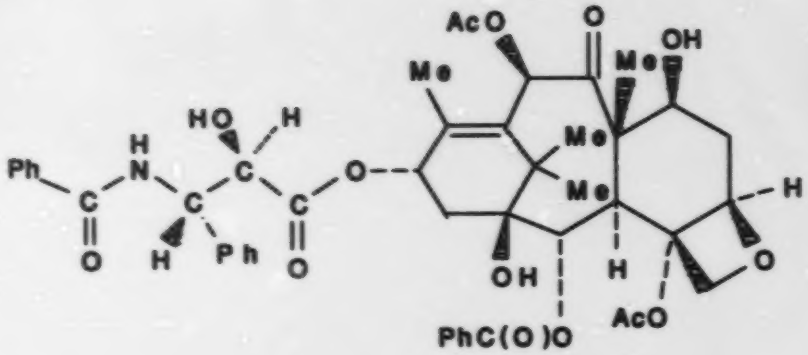
Retention Volumes: 9.5 ml (NSC - 123127)
17.0 ml (I.S.)

Toxicity Data:

Rabbit(iv): LD_{50}: 6.1 mg/kg
Toxicology Branch, NCI

TAXOL

NSC - 125973



Chemical Name:

Benzenepropanoic acid ,β-(benzoylamino)-α-hydroxy-, 6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, [2aR-[2aα,4β,4aβ,6β,9α(αR*,βS*),11α,12α,12aα,12bα]]-

Other Name:

Taxol

Molecular Formula: $C_{47}H_{51}NO_{14}$ **M.W.:** 853.9

Approximate Solubility:

Highly insoluble in water and aqueous solvents. Compound dissolves in methanol, ethanol, benzene, chloroform, methylene chloride, and tetrahydrofuran.

BEST COPY AVAILABLE

Stability:

Bulk:

Bulk samples stored at room temperature for 30 days showed no decomposition as indicated by UV absorption, TLC, or HPLC. The bulk compound stored at 60° C. for three weeks also showed no decomposition. After four weeks very minor decomposition was detected by TLC.

Ultraviolet Absorption:

(MeOH)

$\lambda_{max} = 227 \pm 2$ nm $\varepsilon = 28{,}500 - 30{,}900$

High Performance Liquid Chromatography:

Column: 30 cm x 3.9 mm ID, μPorasil

Mobile Phase: MeOH/CH_2Cl_2/n-hexane/HOAc,
2/20/80/0.01

Flow Rate: 4.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 1.0 mg/0.5 ml in methylene chloride
or internal standard solution

Internal Standard: resorcinol (2 mg/ml in CH_2Cl_2)

Retention Volumes: 44 ml (NSC - 125973)
26 ml (I.S.)

Optical Rotation:

(c = 1, MeOH) $[\alpha]^{20}_{D}$ = -49 to -53°

Toxicity Data:

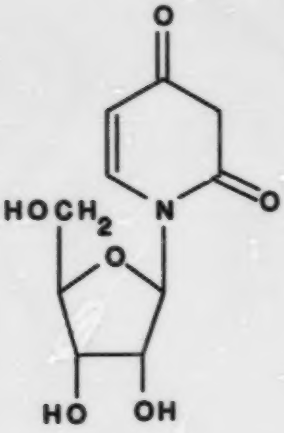
Rat(ip): LD_{50}: 32530 μg/kg
National Technical Information Service, PB83-170969

Mouse(ip): LD_{50}: 128 mg/kg
National Technical Information Service, PB83-170969

Dog(iv): LD_{Lo}: 15 mg/kg
National Technical Information Service, PB83-170969

3-DEAZAURIDINE

NSC - 126849



Chemical Name:
2,4(1H,3H)-Pyridinedione, 1-β-D-ribofuranosyl-

Other Name:
3-Deazauridine

Molecular Formula: $C_{10}H_{13}NO_6$ **M.W.:** 243.2

Approximate Solubility:	(mg/ml)
H_2O	18
DMSO	> 150
EtOH	< 1
DMF	> 150
EtOAc	0.2
$CHCl_3$	0.2

Stability:

Bulk:
A sample stored at 60° C. for 30 days showed no decomposition by UV absorption or paper chromatography.

Solution:
A 2% aqueous solution held at room temperature for 24 hours showed no decomposition by UV absorption or paper chromatography.

Ultraviolet Absorption:

(0.1 N NaOH)

$\lambda_{max} = 255 \pm 2$ nm $\varepsilon = 7{,}850 - 8{,}200$

High Performance Liquid Chromatography:

Column: μBondapak C18, 300 x 4 mm ID

Mobile Phase: pH 4.0 acetate buffer, 0.02 M

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 10 mg/ml in mobile phase or internal standard solution

Internal Standard: uracil (5 mg/ml in mobile phase)

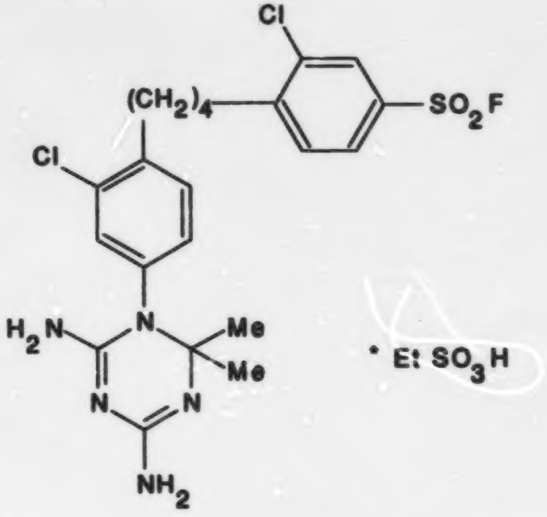
Retention Volume: 17 ml (NSC - 126849)

Optical Rotation:

($c = 1$, H_2O) $[\alpha]^{22}_D = 43.0 \pm 2°$

DIHYDROTRIAZINE BENZENESULFONYL FLUORIDE

NSC - 127755


Cl
(CH2)4
SO2F
Cl
H2N
N
Me
Me
N
N
NH2
• Et SO3H

Chemical Name:
Ethanesulfonic acid, compd. with 3-chloro-4-[4-[2-chloro-4-(4,6-diamino-2,2-dimethyl-s-triazin-1(2H)-yl)phenyl]-butyl]benzenesulfonyl fluoride (1:1)

Other Name:
Dihydrotriazine benzenesulfonyl fluoride

Molecular Formula: $C_{21}H_{24}Cl_2FN_5O_2S \cdot C_2H_5SO_3H$

Molecular Weight: 610.6

Approximate Solubility:	(mg/ml)
TFA	> 200
DMSO	200
MeOH	35
95% EtOH	9.7
H_2O	0.09
10% DMA	3.3

Stability:

Bulk:
As a bulk chemical kept in a screw-capped vial and stored in a 60° C. oven, the sample appeared stable for at least 30 days.(HPLC)

Solution:
A saturated solution in 10% aqueous DMA is stable at room temperature for 24 hours. (HPLC)

Ultraviolet Absorption:

(95% EtOH)

$\lambda_{max} = 235 \pm 2$ nm $\varepsilon = 22{,}500 - 23{,}000$

High Performance Liquid Chromatography:

Column: μPorasil, 28 cm x 3.2 mm ID

Mobile Phase: 10% MeOH in CH_2Cl_2 with 4 x 10^{-4} M
PIC B-7

Flow Rate: 1 ml/min

Detection: UV at 254 nm

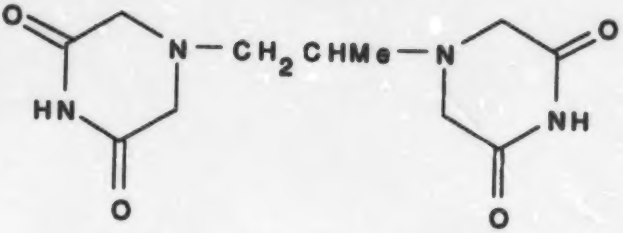
Sample Preparation: 1 mg/ml in methanol or internal
standard solution

Internal Standard: 3,4-diaminobenzoic acid (8 mg/25 ml
methanol)

Retention Volumes: 22.0 ml (NSC - 127755)
12.5 ml (I.S.)

ICRF-159

NSC - 129943



Chemical Name:
2,6-Piperazinedione, 4,4'-propylenedi-, (±)-

Other Names:
ICRF-159; Razoxane

Molecular Formula: $C_{11}H_{16}N_4O_4$ **M.W.:** 268.3

Approximate Solubility:	**(mg/ml)**
Water	3
DMSO 10%	3
DMSO	> 50
Pyridine	> 50
TFA; DMA; DMF	50 - 100
MEK; MeOH; EtOH	< 1

Stability:

Bulk:

No decomposition occurs after 30 days at 60° C. in a glass stoppered bottle, as indicated by TLC.

Solution:

A 3.9 mg/ml solution in 10% DMSO showed no decomposition after 48 hours at room temperature, as indicated by TLC.

High Performance Liquid Chromatography:

Column: Alltech Spherisorb S5 ODS, 25 cm x 4.6 mm ID

Mobile Phase: 5% CH_3CN/H_2O

Flow Rate: 2 ml/min

Detection: UV at 210 nm

Sample Preparation: 1 mg/ml in water or internal standard solution

Internal Standard: tryptophan (2 mg/ml in water)

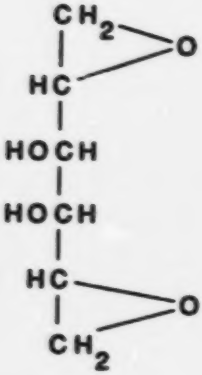
Retention Volumes: 11.4 ml (NSC-129943)
15.0 ml (I.S.)

Toxicity Data:

Human(po): TD_{Lo}: 500 mg/kg
Cancer Treatment Reports, 62,465,(1978)

1,2:5,6-DIANHYDROGALACTITOL

NSC - 132313



Chemical Name:
Galactitol, 1,2:5,6-dianhydro-

Other Names:
DAG; 1,2: 5,6-Dianhydrogalactitol

Molecular Formula: $C_6H_{10}O_4$ **M.W.:** 146.1

Approximate Solubility:	(mg/ml)
H_2O	330
EtOH	30
DMA	500

Stability:

Solution:

A 5% solution has been found to be stable for a 24 hour period at room temperature. No decomposition was detected by either titration or TLC assays.

Gas-Liquid Chromatography:

Column: 10% SP-2100 on 100/120 Supelcoport
1.8 m x 2 mm ID

Carrier Gas: N_2

Flow Rates: N_2, 30 ml/min; H_2, 40 ml/min; air, 300 ml/min

Detector: Flame ionization

Temperatures:		
	Injector	150° C.
	Detector	200° C.
	Oven	100° C.to 210° C. at 10° C./min.

Sample Preparation: The sample (approx. 10 mg) is derivatized by dissolving in 1 ml of BSTFA/pyridine, 1:1, v/v. After standing for 2 hours, the samples are then diluted to 10 ml with internal standard solution.

Internal Standard: hexadecane (0.05µl/ml CH_2Cl_2)

Retention Times: 7.1 min (NSC -132313)
8.6 min (I.S.)

Toxicity Data:

Rat(po): LD_{50}: 14 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

Rat(ip): LD_{50}: 11 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

Rat(iv): LD_{50}: 16 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

Mouse(po): LD_{50}: 17 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

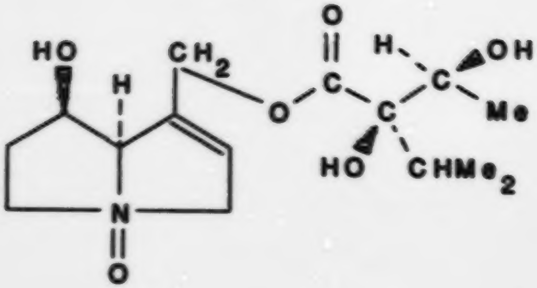
Mouse(ip): LD_{50}: 15 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

Mouse(iv): LD_{50}: 21 mg/kg
Cancer Chemotherapy Reports, 56,593,(1972)

Dog(iv): LD_{Lo}: 16 mg/kg
Cancer Treatment Reports, 60,1585,(1976)

INDICINE N-OXIDE

NSC - 132319



Chemical Name:
Butanoic acid, 2,3-dihydroxy-2-(1-methylethyl)-,(2,3,5,7a-tetrahydro-1-hydroxy-1H-pyrrolizin-7-yl), methyl ester, N-oxide, [1R-(1α,7(2R*,3S*), 7aβ] -

Other Name:
Indicine N-oxide

Molecular Formula: $C_{15}H_{25}NO_6$ **M.W.:** 315.4

Approximate Solubility:	(mg/ml)
H_2O	> 100
Ethanol	> 100
Ethyl Acetate	< 0.02
Chloroform	48

Stability:

Bulk:

A sample stored in a screw cap vial at room temperature showed 1% and 5% decomposition after one week and 31 days respectively. (TLC)

At 60° C., 50% decomposition was detected after nine days. (TLC)

Solution:

A 200 mg/ml solution exposed to laboratory light at room temperature showed no decomposition after 24 hours. (TLC)

Ultraviolet Absorption:

A solution (1 mg/20 ml) does not show any absorption at wavelengths longer than 220 nm.

High Performance Liquid Chromatography:

Column: Zorbax RP-8, 4.6 mm ID x 250 mm

Mobile Phase: $CH_3OH/H_2O/HOAc/Et_3N$, 50/50/0.1/0.02

Flow Rate: 1.0 ml/min

Detection: UV at 206 nm

Sample Preparation: 3 mg/ml in mobile phase or internal standard solution

Internal Standard: propriophenone (10µl/50 ml of mobile phase)

Retention Volumes: 9.0 ml (NSC-132319)
17.0 ml (I.S.)

Optical Rotation:

(c = 1%, EtOH) $[\alpha]^{20}_{D} = +36 \pm 2°$

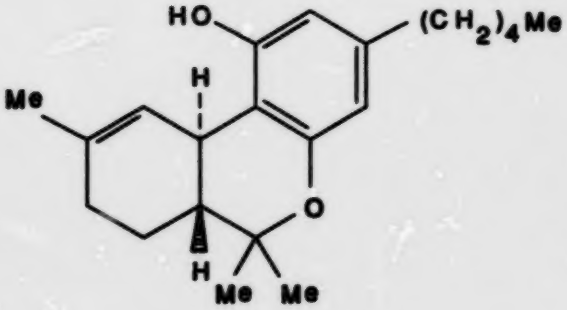
Toxicity Data:

Mouse(iv): LD_{50}: 3733 mg/kg
National Technical Information Service, PB84-161694

Dog(iv): LD_{50}: 1200 mg/kg
Drugs of the Future, 7,633,(1982)

DELTA-9-TETRAHYDROCANNABINOL

NSC - 134454



Chemical Name:
6H-Dibenzo[b,d,]pyran-1-ol, 6a,7,8, 10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, trans-

Other Names:
Delta-9-Tetrahydrocannabinol; Delta-9-THC; THC

Molecular Formula: $C_{21}H_{30}O_2$ **M.W.:** 314.5

Approximate Solubility:
Soluble in acetone, ether, tetrahydrofuran, chloroform, dichloromethane, ethanol.

Ultraviolet Absorption:

(95% Ethanol)

λ_{max}	ε
283 ± 2 nm	1,250 - 1,450
276 ± 2 nm	1,250 - 1,400

High Performance Liquid Chromatography:

Column: 250 mm x 4.6 mm ID Beckman 5 µUltrasphere C18

Mobile Phase: Acetonitrile/1% acetic acid in water, 75:25, v/v

Flow Rate: 1 ml/min

Detection: UV at 280 nm

Sample Preparation: 0.2 mg/ml in internal standard solution

Internal Standard: octanophenone (0.1µl/ml in ethanol)

Retention Volume: 24 ml (NSC-134454)
15 ml (I.S.)

Optical Rotation:

(c = 0.55, $CHCl_3$) $[\alpha]^{25}_D = -170 \pm 3°$

Toxicity Data:

Rat(po): LD_{50}: 666 mg/kg
Proceedings of the Society for Experimental Biology and Medicine, 136,260,(1971)

Rat(ih): LC_{50}: 40 mg/kg
Advances in the Biosciences, 22/23,479,(1979)

Rat(ip): LD_{50}: 373 mg/kg
Proceedings of the Society for Experimental Biology and Medicine, 136,260,(1971)

Rat(iv): LD_{50}: 29 mg/kg
Annals of the New York Academy of Sciences, 191,74,(1971)

Mouse(po): LD_{50}: 482 mg/kg
Proceedings of the Society for Experimental Biology and Medicine, 136,260,(1971)

Mouse(ih) LC_{50}: 40 mg/kg
Advances in the Biosciences, 22/23,479,(1979)

Mouse(ip): LD_{50}: 168 mg/kg
Archives Internationales de Pharmacodynamie et de Therapie, 196,133,(1972)

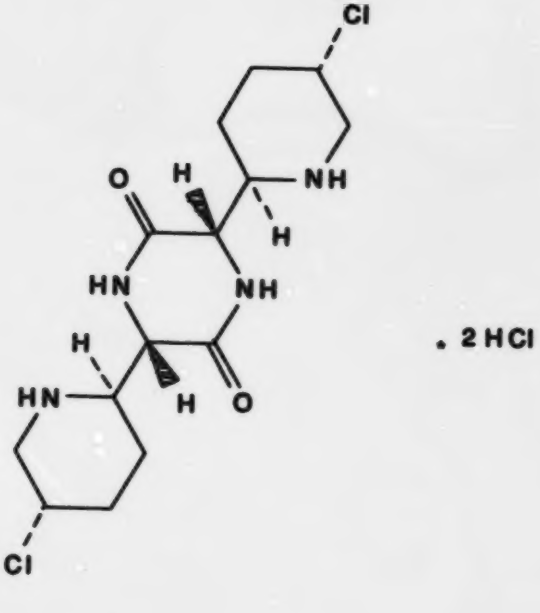
Mouse(iv): LD_{50}: 42 mg/kg
Annals of the New York Academy of Sciences, 191,74,(1971)

Dog(po): LD_{Lo}: 525 mg/kg
Toxicology and Applied Pharmacology, 25,363,(1973)

Monkey(iv): LD_{50}: 128 mg/kg
Toxicology and Applied Pharmacology, 27,648,(1974)

2,5-PIPERAZINEDIONE, 3,6-BIS-(5-CHLORO-2-PIPERIDYL)-, DIHYDROCHLORIDE

NSC - 135758



Chemical Name:
2,5-Piperazinedione; 3,6-bis(5-chloro-2-piperidyl)-, dihydrochloride

Other Names:
Crystalline Antibiotic, Actinomycete Fermentation Product

BEST COPY AVAILABLE

Molecular Formula: $C_{14}H_{22}Cl_2N_4O_2.2HCl$ **M.W.:** 422.2

Approximate Solubility:	(mg/ml)
H_2O	> 100
DMF/H_2O (1:1)	16

Stability:

Bulk:

A sample at 60° C. in a screw-cap vial held for 30 days showed an additional 7 - 8% dehydrohalogenated by-product, and 1 - 2% of hydrolysis products. A sample at room temperature for six months showed no decomposition (paper chromatography).

Protect from air and moisture during storage.

Solution:

A solution of 10 mg/ml water held for 24 hours at room temperature in the light and in the dark showed minimal hydrolysis (estimated less than 1% by paper chromatography).

Ultraviolet Absorption:

(H_2O)

The compound exhibits only end absorption and no discernible maximum in the 210 - 350 nm region.

High Performance Liquid Chromatography:

Column: 3.9 mm ID x 30 cm µBondapak C18

Mobile Phase: 18% acetonitrile in pH 6.7, 0.1 M KH_2PO_4

Flow Rate: 2 ml/min

Detection: UV at 210 nm

Sample Preparation: 20 µg in water

Retention Volume: 19.2 ml (NSC - 135758)

Optical Rotation:

(c = 1.0, H_2O) $[\alpha]^{25}_D = +11 \pm 2°$

Toxicity Data:

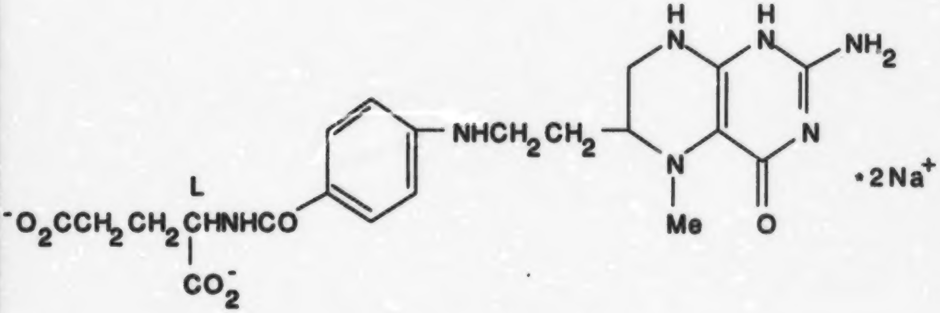
Mouse(ip): LD_{50}: 5 mg/kg
CRC Handbook of Antibiotic Compounds, 4(1),153,(1980)

Mouse(iv): LD_{50}: 19970 µg/kg
National Technical Information Service, PB82-165200

Dog(iv): LD_{50}: 1500 µg/kg
Drugs of the Future, 3,610,(1978)

EMOFOLIN SODIUM

NSC - 139490


H
H
N
N
NH2
N
NHCH2CH2
N
•2Na+
L
-O2CCH2CH2CHNHCO
Me
O
CO2-

Chemical Name:
L-Glutamic acid, N-[4-[[2-(2-amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridinyl)ethyl]amino] benzoyl]-, disodium salt

Other Names:
5-MTHHF; Emofolin Sodium (USAN);
5-Methyltetrahydrohomofolate Disodium; Ketotrexate Sodium

Molecular Formula: $C_{21}H_{25}N_7O_6Na_2$ **M.W.:** 517.5

Approximate Solubility:
Soluble in water (> 100 mg/ml) and slightly soluble in methanol.

Stability:

Bulk:

A sample stored at 30° C. for 30 days showed 15% decomposition as indicated by HPLC.
The compound should be stored in a deep-freeze (-20° C.) protected from air and moisture.

Solution:

The rates of decomposition in neutral and slightly alkaline solutions are comparable and approximately one-half that for slightly acidic solutions. A solution containing 20 mg/ml of the compound and 10 mg/ml ascorbic acid is stable for 24 hours at room temperature.

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 266 \pm 2$ nm $\varepsilon = 14{,}500 - 15{,}300$

High Performance Liquid Chromatography:

Column: 300 mm x 4 mm ID Spherisorb ODS

Mobile Phase: 10% MeOH in 0.1 M KH_2PO_4 pH 6.7;
0.01% dithiothreitol

Flow Rate: 3 ml/min

Detection: UV at 254 nm

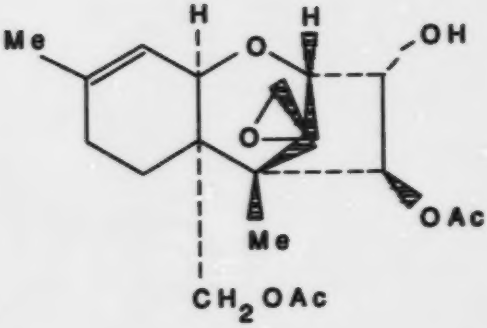
Sample Preparation: 1 mg/ml mobile phase or internal standard solution and adjust pH of final solution to 7

Internal Standard: methotrexate (3.5 mg/10 ml 0.02 N NaOH)

Retention Volume: 17 ml (NSC-139490)
48 ml (I.S.)

ANGUIDINE

NSC - 141537



Chemical Name:
Spiro[2,5-methano-1-benzoxepin-10,2'-oxirane]-5a(6H)-methanol,2,3,4,5,7,9a-hexahydro-3,4-dihydroxy-5,8-dimethyl-, 4,5a-diacetate

Other Names:
Anguidine; Diacetoxyscirpenol;

Molecular Formula: $C_{19}H_{26}O_7$ **M.W.:** 366.4

BEST COPY AVAILABLE

Approximate Solubility:	**(mg/ml)**
Water	1 - 2
5% Dextrose	1 - 2
10% Ethanol	8
10% DMA	10 - 12
10% DMSO	5 - 7
Ethyl acetate	75
Chloroform	> 150
Ethanol	130
DMA	> 300
DMSO	> 100

Stability:

Bulk:

No decomposition was detected by TLC after storage at 60° C. for 30 days.

Solution:

A solution of 5 mg/ml in 10% ethanol which was stored at room temperature for 24 hours showed no decomposition by TLC.

Gas-Liquid Chromatography:

Column: 6 ft, 1/8 in, 10% OV-17 on Anakrom A

Temperatures:		
	Column	220° C.
	Inlet	230° C.
	Detector	290° C.

Detection: Flame ionization

Retention Time: 18 min (NSC - 141537)

Optical Rotation:

(c = 1.30, $CHCl_3$) $[\alpha]^{22}_D = -26.0 \pm 1.0°$

Toxicity Data:

Rat(iv): LD_{50}: 1300 µg/kg
Arzneimittel-Forschung, 18,989,(1968)

Mouse(po): LD_{50}: 7300 µg/kg
CRC Handbook of Antibiotic Compounds, 6,184,(1981)

Mouse(ip): LD_{50}: 20 mg/kg
Toxicologist, 4,12,(1984)

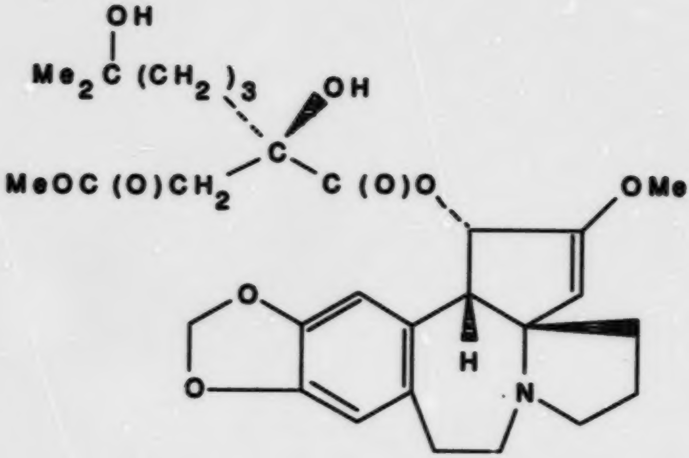
Mouse(iv): LD_{50}: 12400 µg/kg
National Technical Information Service, PB82-166307

Dog(iv): LD_{50}: 1100 µg/kg
Arzneimittel-Forschung 18,989,(1968)

Rabbit(iv): LD_{50}: 1 mg/kg
Arzneimittel-Forschung, 18,989,(1968)

HOMOHARRINGTONINE

NSC - 141633


OH
Me2C (CH2)3
OH
C
MeOC (O)CH2
C (O)O
OMe
O
O
H
N

Chemical Name:
Cephalotaxine, 4-methyl-2-hydroxy-2-(4-hydroxy-4-methylpentyl)butanedioate ester

Other Name:
Homoharringtonine

Molecular Formula: $C_{29}H_{39}NO_9$ **M.W.:** 545.6

BEST COPY AVAILABLE

Stability:

Bulk:

Room temperature and 60° C. stability studies indicate the chemical to be stable for at least 30 days. (HPLC)

Solution:

Room temperature stability studies for homoharringtonine (1 mg/ml) in 10% ethanol showed 16% decomposition after 24 hours and 35% decomposition after 96 hours. (HPLC)

Ultraviolet Absorption:

(Methanol)

$\lambda_{max} = 291 \pm 2$ nm $\varepsilon = 4{,}000 - 4{,}250$

High Performance Liquid Chromatography:

Column: Waters RCM C-18 cartridge

Mobile Phase: MeOH/water/NH_4OH (75/50/3)

Flow Rate: 3 ml/min

Detection: UV at 280 nm

Sample Preparation: 1 mg/ml in methanol or internal standard solution

Internal Standard: strychnine (30 mg/25 ml of MeOH)

Retention Volumes: 12.0 ml (NSC-141633)
5.2 ml (I.S.)

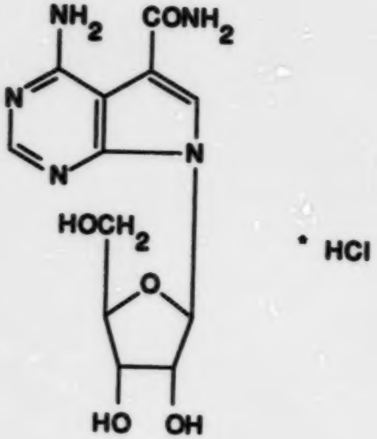
Toxicity Data:

Mouse(ip): LD_{50}: 1960 µg/kg
Chinese Medical Journal, 92,175,(1979)

Mouse(ip): LD50: 6.5 mg/kg
Journal of Applied Toxicology,6,270(1986)

SANGIVAMYCIN HYDROCHLORIDE

NSC - 143648


NH2
CONH2
N
N
N
HOCH2
O
HO
OH
· HCl

Chemical Name:
7H-Pyrrolo[2,3-d]pyrimidine-5-carboxamide,
4-amino-7-β-D-ribofuranosyl-, monohydrochloride

Other Name:
Sangivamycin HCl

Molecular Formula: $C_{12}H_{15}N_5O_5 \cdot HCl$ **M.W.:** 345.7

Approximate Solubility: (mg/ml)

H_2O	~ 1
EtOH	0.5
0.1 N NaOH	< 1
0.1 N HCl	2
DMSO	60
hexane	<< 1
$CHCl_3$	<< 1

Stability:

Bulk:
The compound is stable at room temperature and ordinary laboratory illumination for at least 4 weeks. As a bulk chemical in a capped glass vial and heated at 45° C., the sample is stable for at least 4 weeks. (HPLC)

Solution:
A 1 mg/ml sangivamycin hydrochloride solution in water at room temperature is stable for at least 24 hours as determined by HPLC.

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max}	ε
275 ± 2 nm	11,500 - 11,610
230 ± 2 nm	13,450 - 13,550

High Performance Liquid Chromatography:

Column: μBondapak C18

Mobile Phase: 10% CH_3OH in 0.1 M KH_2PO_4, pH 3.66

Flow Rate: 1 ml/min

Detection: UV at 230 nm

Sample Preparation: 1 mg/ml in 0.1 N HCl or internal standard solution

Internal Standard: adenosine (2.5 mg/ml in 0.1 N HCl)

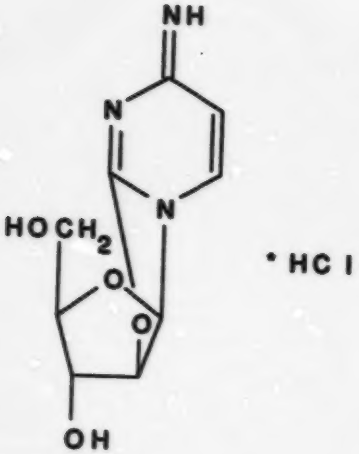
Retention Volumes: 13.5 ml (NSC - 143648)
11.0 ml (I.S.)

Optical Rotation:

(c = 0.1, 0.1 N HCl) $[\alpha]^{20}_{D} = -45 \pm 2°$

CYCLOCYTIDINE HYDROCHLORIDE

NSC - 145668



Chemical Name:
6H-Furo(2',3':4,5)oxazolo(3,2-a)pyrimidine-2-methanol,
2,3,3a,9a-tetrahydro-3-hydroxy-6-imino-,
monohydrochloride

Other Names:
Cyclo-C; Cyclocytidine hydrochloride

Molecular Formula: $C_9H_{11}N_3O_4 \cdot HCl$ **M.W.:** 261.7

Approximate Solubility:

	(mg/ml)
H_2O	200
EtOAc	< 0.1
$CHCl_3$	< 0.1

Stability:

Bulk:

A sample stored at 60° C. for 30 days showed no decomposition as indicated by optical rotation.

Solution:

A 1% solution in water after 24 hours at room temperature showed no decomposition as indicated by optical rotation.

High Performance Liquid Chromatography:

Column: Waters Associates µBondapak C18, 300 x 3.9 mm ID

Mobile Phase: 1.5% acetic acid in water with 0.075 M heptanesulfonic acid

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: Sample concentration - 1.0 mg/ml

Retention Volume: 8.2 ml (NSC-145668)

Ultraviolet Absorption:

(H_2O)

λ_{max}	ε
231 ± 2 nm	9,300 - 9,700
263 ± 2 nm	10,400 - 10,800

Optical Rotation:

($c = 2, H_2O$) $[\alpha]^{20}_D = -22 \pm 2°$

Toxicity Data:

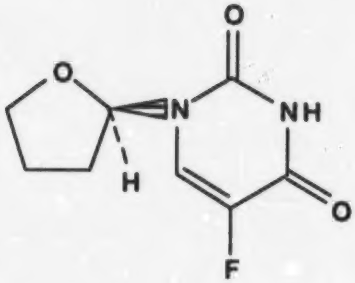
Mouse(iv): LD_{50}: 800 mg/kg
Drugs in Japan. Ethical Drugs, 6,55,(1982)

Dog(iv): LD_{50}: 344 mg/kg
Oyo Yakuri. Pharmacometrics, 8,353,(1974)

Monkey(iv): LD_{50}: 1045 mg/kg
Oyo Yakuri. Pharmacometrics, 8,353,(1974)

TEGAFUR

NSC - 148958



Chemical Name:
Uracil, 5-fluoro-1-(tetrahydro-2-furyl)-

Other Names:
Ftorafur; FT-203; Tegafur (USAN)

Molecular Formula: $C_8H_9N_2O_3F$ **M.W.:** 200.2

Approximate Solubility:	(mg/ml)
Dimethyl Sulfoxide	> 200
Chloroform	30
0.1 N NaOH	33.5
0.1 N HCl	10
Water	9
pH 7 buffer	6
Ethanol	6

Stability:

Bulk:

A sample stored 30 days at 60° C. showed no decomposition as indicated by paper chromatography and UV absorption.

Solution:

A solution of the compound at pH 9.5, and stored for 24 hours at room temperature, showed no decomposition as indicated by paper chromatography or UV absorption. The solution was prepared by dissolving 80 mg of the compound and 10 mg anhydrous sodium carbonate in 1.6 ml of 0.2 N NaOH and 0.4 ml water.

Ultraviolet Absorption:

(pH 7 buffer)

$\lambda_{max} = 271 \pm 2$ nm $\qquad \varepsilon = 8{,}550 - 8{,}850$

High Performance Liquid Chromatography:

Column: Waters C18 μBondapak, 10m,
300 x 3.9 mm ID

Mobile Phase: CH_3CN/1% HOAc (aq), 10/90, v/v

Flow Rate: 1.0 ml/min

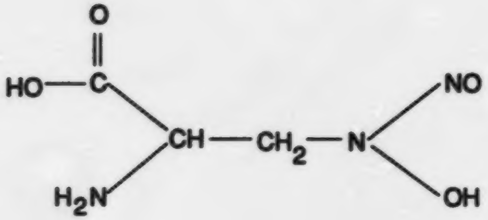
Detection: UV at 254 nm

Sample Preparation: Sample concentration - 0.1 mg/ml

__Retention Volume__: 9.7 ml (NSC -148958)

L-ALANOSINE

NSC-153353



Chemical Name:
Propionic acid, L-2-amino-3-(hydroxy-nitrosoamino)-

Other Name:
L-Alanosine

Molecular Formula: $C_3H_7N_3O_4$ **M.W.:** 149.1

Approximate Solubility:	(mg/ml)
CH_3OH	< 0.1
CH_2Cl_2	< 0.1
95% Ethanol	< 0.1
$CHCl_3$	< 0.1
H_2O	0.7 - 1.0
0.1 N HCl	6 - 7

Stability:

Bulk:

A sample stored at room temperature under air for 7 months showed 8-10% decomposition. A sample stored at room temperature under nitrogen showed 2% decomposition.

Store bulk compound under nitrogen or argon in the refrigerator.

Solution:

Solutions in 0.1N HCl (pH 1.0 ± 0.05), 0.1N NaOH (pH 12.8 ± 0.2) and in deionized water (pH 3.8 ± 0.05) ranging in concentration from 1 - 1.7 mg/ml, were all found to be stable at room temperature for at least 24 hours by UV and optical rotation analyses.

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 228 \pm 2$ nm $\varepsilon =$ 6,500 - 7,500

High Performance Liquid Chromatography:

Column: Zorbax NH_2 with SAX guard column

Mobile Phase: 0.1 M pH 2.5 acetate buffer

Flow Rate: 1 ml/min

Detection: UV at 228 nm

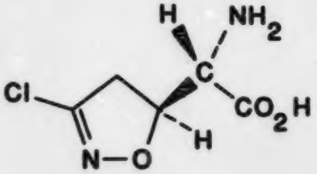
Retention Volume: 9 ml (NSC-153353)

Optical Rotation:

(c = 1, 0.1 N NaOH) $[\alpha]^{20}_{D} = -39 \pm 2°$

ACIVICIN

NSC-163501



Chemical Name:

5-Isoxazoleacetic acid, α-amino-3-chloro-4,5-dihydro-

Other Names:

AT-125; U-42126; Acivicin (USAN)

Molecular Formula: $C_5H_7ClN_2O_3$ **M.W.:** 178.6

Approximate Solubility:	**(mg/ml)**
Water	17.9 - 18.2
0.1 M Citrate buffer pH 4.3	17.1 - 25.7
0.1 M Borate buffer pH 9.0	8.7 - 13.0
0.1 N HCl	31 - 35
0.1 N NaOH	34.4 - 36.8
95% Ethanol	0.8
10% Ethanol	8.2 - 16.4
Methanol	0.8
Chloroform	0.9

BEST COPY AVAILABLE

Stability:

Bulk:

A sample stored at 60° C. for 14 days showed no decomposition as indicated by UV absorption, paper chromatography, or ionic chloride determination.

Solution:

An aqueous solution (18 mg/ml) which was stored at 28° C. for 14 days showed less than 1% decomposition by UV absorption, paper chromatography and ionic chloride measurement.

Ultraviolet Absorption:

(H_2O)

$\lambda_{max} = 218 \pm 2$ nm $\varepsilon = 3{,}500 - 3{,}700$

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18
300 x 3.9 mm ID

Mobile Phase: Water containing 0.0075 M heptane sulfonic acid, pH 2.5

Flow Rate: 1.0 ml/min

Detection: UV at 218 nm

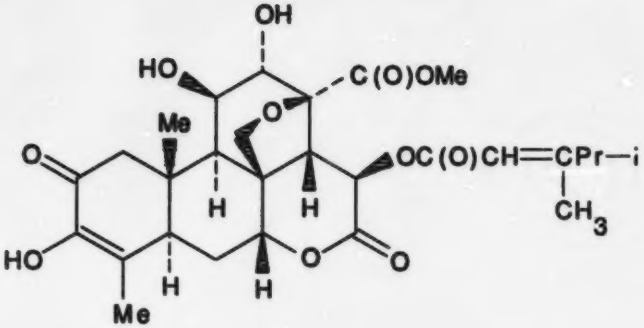
Sample Preparation: 1.0 mg/ml in water or internal standard solution

Internal Standard: nicotinic acid (0.825 mg/ml in water)

Retention Volumes: 5.4 ml (NSC-163501)
7.8 ml (I.S.)

BRUCEANTIN

NSC- 165563


OH
HO
C(O)OMe
O
Me
O
OC(O)CH=CPr—i
CH3
H
H
HO
O
O
H
H
Me

Chemical Name:
Picras-3-en-21-oic acid, 15-[(3,4-dimethyl-1-oxo-2-pentenyl)oxy]-13,20-epoxy-3,11,12-trihydroxy-2,16-dioxo-, methyl ester, [11β,12α,15β(E)]-

Other Name:
Bruceantin

Molecular Formula: $C_{28}H_{36}O_{11}$ **M.W.:** 548.6

Approximate Solubility:	(mg/ml)
H_2O	< 0.01
10% Glycerin	< 0.01
10% Ethanol	< 0.01
Absolute Ethanol	8

BEST COPY AVAILABLE

Stability:

Bulk:

A sample of the bulk chemical stored in a screw cap bottle for 18 days at 60° C. showed no decomposition as indicated by TLC.

Solution:

A solution of 2.5 mg in 10 ml 10% ethanol showed no decomposition after 5 hours and less than 1% decomposition after 24 hours as indicated by TLC.

Ultraviolet Absorption:

(95% Ethanol)

λ_{max}	ε
221 ± 2 nm	17,100 - 17,600
280 ± 2 nm	8,820 - 8,930

High Performance Liquid Chromatography:

Column: 300 mm x 4 mm ID Spherisorb ODS

Mobile Phase: pH 6.7, 0.1 M KH_2PO_4/CH_3OH, 1/1

Flow Rate: 2 ml/min

Detection: UV at 280 nm

Sample Preparation: 0.8 mg/ml in methanol or internal standard solution

Internal Standard: naphthalene (1 mg/ml in methanol)

Retention Volumes: 11 ml (NSC-165563)
30 ml (I.S.)

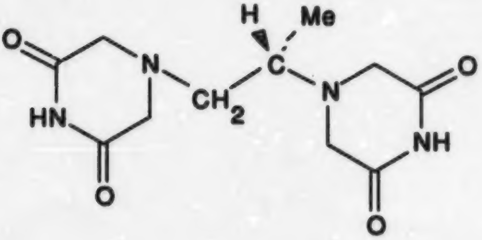
Toxicity Data:

Mouse(iv): LD_{50}: 1950 μg/kg
Toxicology and Applied Pharmacology, 41,192,(1977)

Dog(iv): LD_{Lo}: 500 μg/kg
Toxicology and Applied Pharmacology, 41,192,(1977)

ICRF-187

NSC- 169780



Chemical Name:
2,6-Piperazinedione, 4,4’-(1-methyl-1,2-ethanediyl)bis-,(+)-

Other Name:
ICRF-187

Molecular Formula: $C_{11}H_{16}N_4O_4$ **M.W.:** 268.3

Approximate Solubility:	(mg/ml)
H_2O	10 - 12
0.1 N HCl	35 - 43
0.1 N NaOH	25 - 34
10% EtOH	6.7 - 10
MeOH	1
H_20/DMA (1:1)	7.1 - 10
0.1 M Citrate Buffer (pH 4)	9.7 - 14.5
0.1 M Borate Buffer (pH 9)	8.7 - 13

Stability:

Bulk:

A sample stored at 60° C. showed less than 1% decomposition after seven days as indicated by HPLC.

Solution:

A 10 mg/ml solution in water at 28° C. showed 10% and 42% decomposition in 1 day and 6 days respectively as indicated by HPLC.

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18
300 x 3.9 mm ID

Mobile Phase: CH_3CN/pH 7 0.01 M phosphate buffer,
10/90, v/v

Flow Rate: 1 ml/min

Detection: UV at 200 nm

Sample Preparation: 0.05 mg/ml in internal standard
solution

Internal Standard: acetanilide (0.08 mg/ml in
acetonitrile/0.01 M phosphate
buffer, pH 7, 3.5/96.5, v/v)

Retention Volumes: 6.6 ml (NSC-169780)
19.5 ml (I.S.)

Optical Rotation:

(c = 0.5, H_2O) $[\alpha]^{26}_D = +42 \pm 2°$

Toxicity Data:

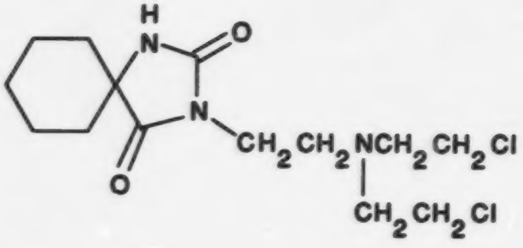
Man(iv): TD_{Lo}: 383 mg/kg
Cancer Clinical Trials, 4,143,(1981)

Mouse(ip): LD_{Lo}: 800 mg/kg
Drugs of the Future, 2,473,(1977)

Dog(iv): LD_{Lo}: 2 gm/kg
Cancer Treatment Reports, 64,1211,(1980)

SPIROMUSTINE

NSC- 172112



Chemical Name:
1,3-diazaspiro[4.5]decane-2,4-dione,
3-[2-[bis(2-chloroethyl)amino]ethyl]-

Other Names:
Spiromustine (USAN), Spirohydantoin mustard

Molecular Formula: $C_{14}H_{23}Cl_2N_3O_2$ **M.W.:** 336.3

Approximate Solubility:	**(mg/ml)**
H_2O	< 0.01
5% Urea	< 0.1
5% Dextrose, pH 4	< 0.1
10% Ethanol	0.03
10% DMA	0.35
10% DMF	0.33
10% DMSO	0.30

Stability:

Bulk:

The bulk compound is stable at 60° C. for 30 days as indicated by TLC and ionic chloride determinations.

Solution:

Saturated solutions in 10% DMA adjusted to pH 5 had a half-life between 30 and 60 minutes, as indicated by ionic chloride determination.

Ultraviolet Absorption:

(95% Ethanol)

The ultraviolet absorption spectrum shows no absorption maxima other than the expected end absorption.

High Performance Liquid Chromatography:

Column: 250 mm x 4.6 mm ID Zorbax SIL

Mobile Phase: 14% THF in n-hexane

Flow Rate: 2.0 ml/min

Detection: UV at 225 nm

Sample Preparation: 6 mg samples are dissolved in 2.0 ml internal standard solution

Internal Standard: o-nitroaniline (0.025 mg/ml in THF)

Retention Volume: 23.2 ml (NSC-172112)
9.0 ml (I.S.)

Gas-Liquid Chromatography:

Column: 3% OV-1 (6 ft x 2 mm)

Carrier Gas: N_2

Flow Rate: 35 ml/min

Temperatures: Column 200° C.
Detector 250° C.
Inlet 250° C.

Detection: FID

Retention Time: 5 min (NSC-172112)

Toxicity Data:

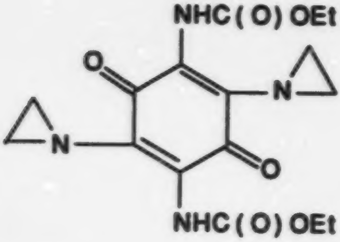
Rat(iv): LD_{50}: 9100 µg/kg
National Technical Information Service, PB83-149518

Mouse(iv): LD_{50}: 48280 µg/kg
National Technical Information Service, PB83-148395

Dog(iv): LD_{Lo}: 3750 µg/kg
National Technical Information Service, PB83-149518

DIAZIQUONE

NSC- 182986



Chemical Name:
1,4-Cyclohexadiene-1,4-dicarbamic acid, 2,5-bis(1-aziridinyl)-3,6-dioxo-, diethyl ester

Other Names:
AZQ; Aziridinylbenzoquinone; Diaziquone (USAN)

Molecular Formula: $C_{16}H_{20}N_4O_6$ **M.W.:** 364.4

Approximate Solubility:	(mg/ml)
Water	0.72
pH 4 buffer	< 1
pH 9 buffer	< 1
10% Ethanol	< 1
95% Ethanol	< 1
Methanol	< 1
Chloroform	5 - 7
5% Dimethylacetamide	1.5
Dimethylacetamide	20 - 25
Dimethylsulfoxide	25 - 30

Stability:

Bulk:

A sample stored at 60° C. in the dark for 30 days showed < 2% decomposition as indicated by HPLC.

Solution:

A sample in 5% DMA (1 mg/ml) showed 18% decomposition after 8 hours at room temperature. (HPLC)

Ultraviolet Absorption:

(Methanol)

$\lambda_{max} = 217 \pm 2$ nm	$\varepsilon = 22,200 - 22,800$
$\lambda_{max} = 341 \pm 2$ nm	$\varepsilon = 13,900 - 14,300$

High Performance Liquid Chromatography:

Column: μBondapak Phenyl, 300 x 4 mm ID

Mobile Phase: CH_3CN/0.01 M pH 7 phosphate, 15/85, v/v

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: Sample solvent CH_3CN

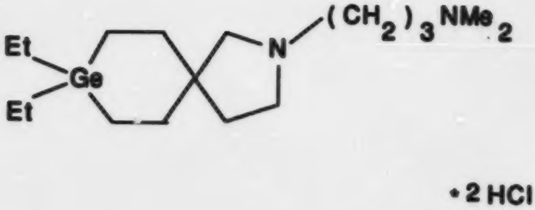
Retention Volume: 15 ml (NSC-182986)

Toxicity Data:

Mouse(iv): LD_{50}: 10300 µg/kg
National Technical Information Service, PB80-177934

SPIROGERMANIUM HYDROCHLORIDE

NSC- 192965



Chemical Name:

2-Aza-8-germaspiro(4.5)decane-2-propanamine, 8,8-diethyl-N,N-dimethyl-, dihydrochloride

Other Names:

Spiro-32; Spirogermanium Hydrochloride (USAN)

Molecular Formula: $C_{17}H_{36}GeN_2 \cdot 2HCl$ **M.W.:** 414.0

Approximate Solubility:	(mg/ml)
Water	> 50
pH 4 buffer	> 30
pH 9 buffer	> 30
Methanol	> 25
Benzene	< 1
Chloroform	6-10
95% Ethanol	> 28

Stability:

Bulk:

A sample stored at 60° C. showed no decomposition as indicated by GLC and TLC through 30 days.

Solution:

The compound was dissolved in D_2O at 50 mg/ml concentration. No decomposition was detected by NMR or TLC after 7 days at room temperature.

Gas-Liquid Chromatography:

Column: 3% SP-2250-DB on 100/120 Supelcoport, 1.8 m x 4 mm ID

Carrier Gas: N_2

Flow Rates: N_2, 30 ml/min; H_2, 30 ml/min; and air, 300 ml/min

Detection: Flame ionization

Temperatures:		
	Column	195° C.
	Injector	250° C.
	Detector	220° C.

Sample Preparation: 20 mg/25 ml internal standard solution

Internal Standard: fluoranthrene (0.8 mg/ml in 0.9% saline/methanol, 1/11, v/v. Each solution contains three KOH pellets).

Retention Times: 5.5 min (NSC - 192965)
11.5 min (I.S.)

Toxicity Data:

Mouse(iv): LD_{50}: 41500 µg/kg
National Technical Information Service, PB264-117

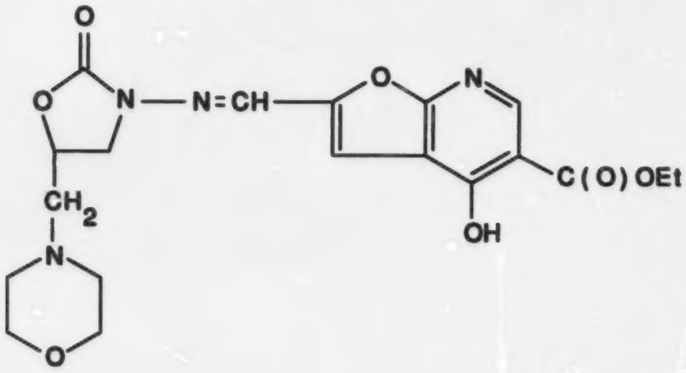
Mouse(im): LD_{50}: 119 mg/kg
Cancer Treatment Reports, 64,1207,(1980)

Dog(iv): LD_{Lo}: 40 mg/kg
Cancer Treatment Reports, 64,1207,(1980)

Dog(im): LD_{Lo}: 40 mg/kg
Cancer Treatment Reports, 64,1207,(1980)

EBIFURAMIN

NSC - 201047



Chemical Name:
Furo[2,3-b]pyridine-5-carboxylic acid, 4-hydroxy-2-[[[5-(4-morpholinylmethyl)-2-oxo-3-oxazolidinyl]imino]methyl]-, ethyl ester

Other Name:
Ebifuramin

Molecular Formula: $C_{19}H_{22}N_4O_7$ **M.W.:** 418.4

Approximate Solubility:	**(mg/ml)**
H_2O	< 0.62
Buffer, pH 4	< 0.69
Buffer, pH 9	2.0-2.5
EtOH	≤ 0.68
Dimethylacetamide	2.0-2.5
DMSO	5.0-10.0
$CHCl_3$	≥ 10.5
Ethyl acetate	≤ 0.67
t-Butanol	≤ 0.72
CH_3CN	1.47-1.72

Stability:

Bulk:

Samples stored for 3 months under light and dark conditions at 25° C. showed no change. Samples stored at 50° C. in the dark were unchanged.

Ultraviolet Absorption:

(CH_3CN)

λ_{max}	ε
192 ± 2 nm	17,433 ± 200
227 ± 2 nm	16,496 ± 200
244 ± 2 nm	17,189 ± 200
299 ± 2 nm	23,096 ± 200
254 ± 2 nm	14,006 ± 200

High Performance Liquid Chromatography:

Column: RCM 100 Nova Pak C-18 with a 5 µ
RP-18 guard column, 30 x 4.6 mm ID

Mobile Phase: 15% CH_3CN in 0.015 Dibutylamine phosphate,
pH at 2.6

Flow Rate: 2 ml/min

Detection: UV at 254 nm

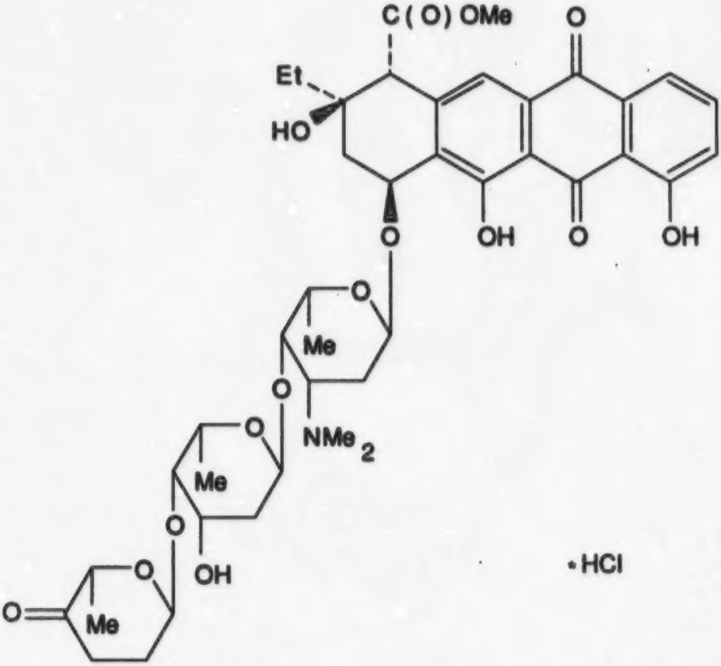
Sample Preparation: 1.0 mg/ml of sample, 0.5 mg/ml internal sta
in CH_3CN

Internal Standard: Acetophenone in CH_3CN (0.5 mg/ml)

Retention Volume: 8.3 ml (NSC 201047)
20.3 (I.S.)

ACLARUBICIN HYDROCHLORIDE

NSC- 208734



Chemical Name:
1-Naphthacenecarboxylic acid, 2-ethyl-1,2,3,4,6,11-hexahydro-2,5,7-trihydroxy-6,11-dioxo-4-[[2,3,6-trideoxy-4-O-[2,6-dideoxy-4-O-[(2R-trans)-tetrahydro-6-methyl-5-oxo-2H-pyran-2-yl]-α-L-lyxo-hexopyranosyl]-3-(dimethylamino)-α-L-lyxo-hexopyranosyl]oxy]-, methyl ester, [1R-(1α,2β,4β)]-, hydrochloride

Other Names:
Aclacinomycin A Hydrochloride; Aclarubicin Hydrochloride

BEST COPY AVAILABLE

(USAN)

Molecular Formula: $C_{42}H_{53}NO_{15}\cdot HCl$ **M.W.:** 848.3

Approximate Solubility: (mg/ml)

Aclacinomycin A, free base

H_2O	< 0.1
0.1 M Na_2CO_3	unstable
0.1 M $NaHCO_3$	< 0.01
10% EtOH	0.1 - 0.2
20% EtOH	< 0.5
95% EtOH	> 200

Stability:

Aclacinomycin A, free base

Bulk:

As a bulk chemical, the sample appears stable for two weeks when stored in a closed container, at room temperature, and in darkness. After four weeks less than 0.5% decomposition. When stored similarly at 60° C. for 4 weeks, the sample decomposes slowly and gradually at a rate of approximately 0.5% per week. (TLC)

Solution:

Because of the poor solubility of the free base, the solution stability was not performed. Based on the TLC and HPLC data, the compound is slightly unstable in acids and less stable in alkali.

Ultraviolet Absorption:

(0.1 N HCl) (Calculated as the anhydrous free base)

λ_{max}	$\varepsilon^1{}_1$
227 ± 2 nm	480 - 520
257 ± 2 nm	310 - 345
435 ± 2 nm	130 - 160

High Performance Liquid Chromatography:

Column: Waters Radial Pak Silica

Mobile Phase: $CHCl_3/MeOH/HOAc/H_2O/Et_2NH$,
68/20/10/2/0.01

Flow Rate: 1.3 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.2 mg/ml in methanol or
internal standard solution

Internal Standard: MA144MI (0.2 mg/ml in methanol)

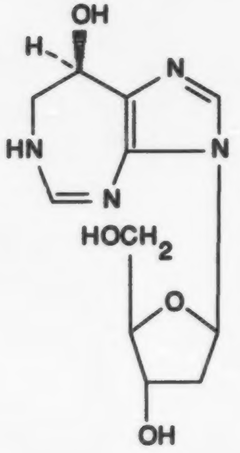
Retention Volume: 13 ml (NSC-208734)
19.5 ml (I.S.)

Optical Rotation:

(C = 1, 0.1 N HCl) $[\alpha]^{20}_D = -165 \pm 5°$

PENTOSTATIN

NSC- 218321



Chemical Name:
Imidazo(4,5-d)[1,3]diazepin-8-ol, 3-(2-deoxy-β-D-erythro-pentofuranosyl)-3,6,7,8-tetrahydro-, (R)-

Other Names:
2'-Deoxycoformycin; Co-Vidarabine; Pentostatin (USAN)

Molecular Formula: $C_{11}H_{16}N_4O_4$ **M.W.:** 268.3

Approximate Solubility:	**(mg/ml)**
H_2O	> 30
pH 9 borate buffer	> 50

Stability:

Bulk:

Bulk samples stored at 60° C. for 9 days showed no decomposition, as indicated by TLC and UV absorption.

Bulk material should be stored at -20° C.

Ultraviolet Absorption:

(pH 9 borate buffer)

$\lambda_{max} = 283 \pm 2$ nm $\varepsilon = 7{,}950 - 8{,}250$

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18
300 x 3.9 mm ID

Mobile Phase: CH_3OH/0.01 M phosphate buffer (pH 7), 13/87, v/v

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.1 mg/ml in internal standard solution

Internal Standard: acetanilide (0.3 mg/ml in mobile phase)

Retention Volume: 7.2 ml (NSC 218321)
28 ml (I.S.)

Optical Rotation:

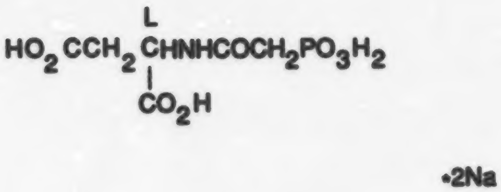
(c = 1, H_2O) $[\alpha]^{25}_D = +76.4 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 122 mg/kg
National Technical Information Service, PB84-211424

PALA DISODIUM

NSC- 224131



$$HO_2CCH_2\underset{\substack{|\\ CO_2H}}{\overset{L}{C}}HNHCOCH_2PO_3H_2 \quad \cdot 2Na$$

Chemical Name:
L-Aspartic acid, N-(phosphonoacetyl)-, disodium salt

Other Names:
N-Phosphonoacetyl-L-Aspartate Disodium; PALA Disodium

Molecular Formula: $C_6H_8NO_8P \cdot 2Na$ **M.W.:** 299.1

Approximate Solubility:	(mg/ml)
Water	> 950

Stability:

Bulk:
The compound is very stable as the bulk drug. The bulk material is hygroscopic; protect from moisture when storing.

Solution:

The compound is very stable as the aqueous solution.

High Performance Liquid Chromatography:

Column: Partisil PXS 10/25 SAX, 250 mm x 4.6 mm ID

Mobile Phase: 0.30 M KH_2PO_4, adjusted to pH 4.0 with H_3PO_4

Flow Rate: 2.0 ml/min

Detection: UV at 210 nm

Sample Preparation: 2 mg/ml in water or internal standard solution

Internal Standard: 1-naphthol-4-sulfonic acid, Na salt (2 mg/50 ml of water)

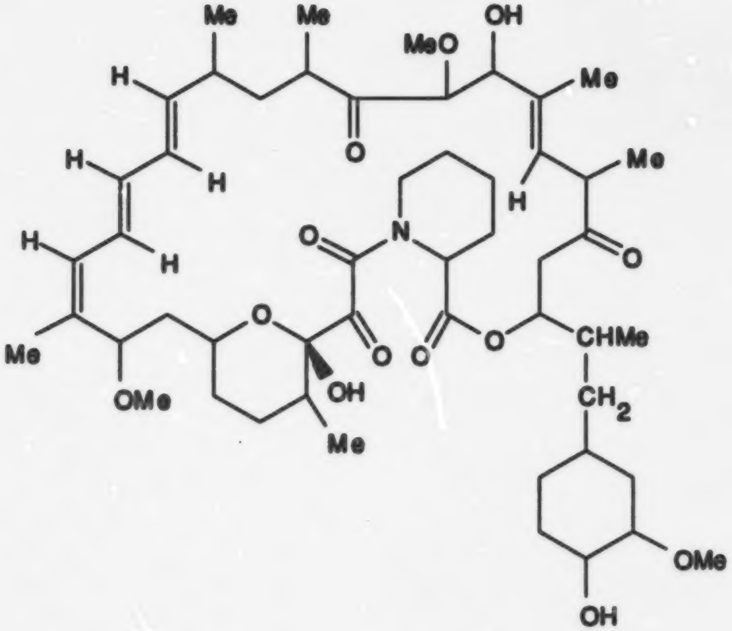
Retention Volume: 10.8 ml (NSC-224131)

Optical Rotation:

(C = 1, H_2O) $[\alpha]^{20}_D = +14.2 \pm 2°$

RAPAMYCIN

NSC- 226080


Me
Me
MeO
OH
H
Me
H
O
Me
H
H
H
O
N
H
O
H
O
Me
O
O
O
CHMe
OH
OMe
CH$_2$
Me
OMe
OH

Name:
Rapamycin

Molecular Formula: $C_{51}H_{79}NO_{13}$ **M.W.:** 914.2

BEST COPY AVAILABLE

Approximate Solubility:

	(mg/ml)
$CHCl_3$	> 50
CH_3OH	> 50
95% Ethanol	15 - 20
10% Ethanol	< 1
H_2O	< 1
pH 4 Acetate buffer	< 1
pH 9 Carbonate buffer	< 1

Stability:

Bulk:

A sample stored at 60° C. in the dark for 30 days showed no decomposition as indicated by HPLC.

Solution:

After storage of a solution (5 mg/ml in 10% ethanol - 10% Cremophor EL-80% sterile water) for 48 hours at room temperature and exposed to lab light, the rapamycin concentration was 98.5% of the zero-time value. (HPLC)

Ultraviolet Absorption:

(95% ethanol)

λ_{max}	ε
289 ± 2 nm	38,070 - 42,400
277 ± 2 nm	50,240 - 56,100
267 ± 2 nm	38,430 - 43,100

High Performance Liquid Chromatography:

Column: Beckman Ultrasphere ODS, 5 µ, 250 mm
x 4.6 mm, ID

Mobile Phase: 0.01 M acetate buffer, pH 5/methanol
(18/82, v/v)

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.5 mg/ml in ethanol containing
internal standard (0.38 mg hexaphenone/ml ethanol)

Retention Volume: 18.3 ml (NSC-226080)
8.4 ml (I.S.)

Toxicity Data:

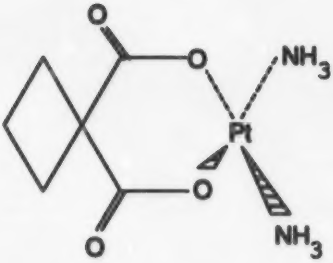
Rat(ip): LD_{50}: 18220 µg/kg
National Technical Information Service, PB83-228577

Mouse(po): LD_{50}: 2500 mg/kg
Antibiotics: Origin, Nature and Properties, 2,947,(1978)

Mouse(ip): LD_{50}: 597 mg/kg
Journal of Anhtibiotics, 31,539,(1978)

CARBOPLATIN

NSC- 241240



Chemical Name:
Platinum, diammine[1,1-cyclobutanedicarboxylato(2-)-O,O']-, (SP-4-2)-

Other Names:
Carboplatin (USAN); CBDCA

Molecular Formula: $C_6H_{12}N_2O_4Pt$ **M.W.:** 371.3

BEST COPY AVAILABLE

Approximate Solubility:	(mg/ml)
Water	> 15
pH 4 Acetate Buffer	5 - 10
pH 9 Carbonate Buffer	5 - 10
10% Ethanol/H_2O	5 - 10
95% Ethanol/H_2O	< 1
0.1 N HCl	5 - 10
0.1 N NaOH	5 - 10
Methanol	< 1
Chloroform	< 5
Dimethylsulfoxide	5
Acetic Acid	< 1
Trifluoroacetic Acid	< 1

Stability:

Bulk:

No decomposition was detected after 30 days at 60° C. in the dark (HPLC).

Solution:

After 48 hours at room temperature an aqueous solution showed < 1% decomposition (HPLC).

High Performance Liquid Chromatography:

Column: Unimetrics LiChrosorb RP -8,
250 x 4.6 mm ID

Mobile Phase: Water

Flow Rate: 1.0 ml/min

Detection: UV at 205 nm

Sample Preparation: About 0.6 mg/ml in water
containing internal standard
(0.11 mg uracil/ml water)

Retention Volumes: 6.2 ml (NSC-241240)
5.5 ml (I.S.)

Toxicity Data:

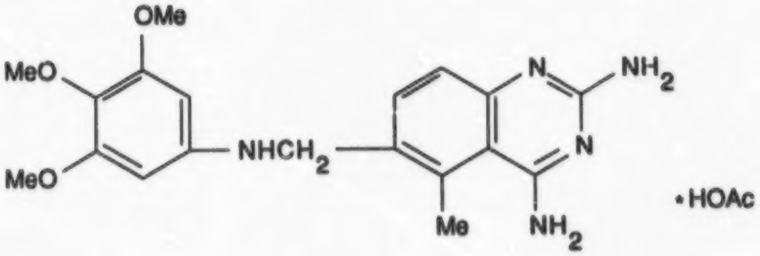
Rat(iv): LD_{50}: 61 mg/kg
Journal of the National Cancer Institute, 67,201,(1981)

Mouse(ip): LD_{Lo}: 150 mg/kg
Bioinorganic Chemistry, 2,187,(1973)

Mouse(iv): LD_{50}: 143 mg/kg
National Technical Information Service, PB82-165028

JB-11

NSC- 249008


OMe
MeO
MeO
NHCH2
N
NH2
N
Me
NH2
•HOAc

Chemical Name:
2,4-Quinazolinediamine,
5-methyl-6-[[(3,4,5-trimethoxyphenyl)amino]methyl]-,
monoacetate

Other Name:
JB-11 (Acetate Salt)

Molecular Formula: $C_{19}H_{23}N_5O_3 \cdot CH_3COOH$ **M.W.:** 429.5

Approximate Solubility: (mg/ml)

Water	1 - 2
pH 4 Acetate buffer	< 1
pH 9 Acetate buffer	< 1
0.1 N HCl	1 - 5
0.1 N NaOH	< 1
Methanol	12 - 15
95% Ethanol	1 - 5
10% Ethanol	1 - 3
Dimethylacetamide	10 - 15
Dimethylsulfoxide	~ 100

Stability:

Bulk:

A sample stored at 60° C. for 30 days showed no decomposition as indicated by UV absorption or HPLC.

Solution:

A solution in 5% methanol (0.5 mg/ml) showed no decomposition after 9 days as indicated by UV absorption. A solution in 5% dimethylacetamide/ pH 4 acetate buffer showed no decomposition after 48 hours, as indicated by HPLC.

Ultraviolet Absorption:

(0.1 N NaOH)

λ_{max}	ε
237 ± 2 nm	46,970 - 47,922

341 ± 2 nm	4,410 - 4,680

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak C18
300 x 3.9 mm ID

Mobile Phase: CH_3CN/3% acetic acid in water,
20/80, v/v

Flow Rate: 0.8 ml/min

Detection: UV at 254 nm

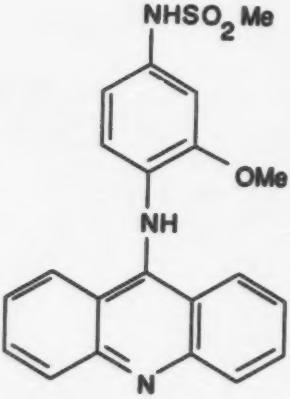
Sample Preparation: 0.5 mg/ml in Methanol containing
internal standard

Internal Standard: 0.35 ml/ml acetophenone in methanol

Retention Volumes: 6.4 ml (NSC-249008)
9.1 ml (I.S.)

AMSACRINE

NSC- 249992



Chemical Name:
Methanesulfonamide, N-[4-(9-acridinylamino)-3-methoxyphenyl]-

Other Names:
m-AMSA; Acridinyl anisidide; Methanesulfon-m-anisidide, 4'-(9-acridinylamino)-; Amsacrine (USAN)

Molecular Formula: $C_{21}H_{19}N_3O_3S$ **M.W.:** 393.5

Approximate Solubility:

	(mg/ml)
Water	< 1.0
pH 4 buffer	< 1.0
pH 9 buffer	< 1.0
10% EtOH	< 1.0
95% EtOH	1.5 - 1.8
MeOH	2.9 - 3.2
$CHCl_3$	1.0

Stability:

Bulk:

A sample stored at 60° C. for 30 days showed no decomposition as indicated by IR, TLC or UV.

Solution:

A sample was dissolved in methanol and diluted with water (1:33). No decomposition was detected by UV after standing 4 days at room temperature and exposed to light.

Ultraviolet Absorption:

(pH 4 Acetate buffer)

λ_{max}	ε
265 ± 2 nm	48,400 - 49,000
430 ± 2 nm	13,050 - 13,250

High Performance Liquid Chromatography:

Column: Waters Associates μBondapak
C18, 300 x 4 mm ID

Mobile Phase: CH_3CN/3% acetic acid in water,
65/35, v/v

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.2 mg/ml in methanol
containing internal standard

Internal Standard: 0.2μl hexaphenone/ml of methanol

Retention Volume: 6.0 ml (NSC-249992)

Toxicity Data:

Human(iv): TD_{Lo}: 12 mg/kg
Cancer Research, 38,3712,(1978)

Mouse(po): LD_{50}: 53420 μg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 15470 μg/kg
NCI Screening Program Data Summary

Mouse(sc): LD_{50}: 110 mg/kg
NCI Screening Program Data Summary

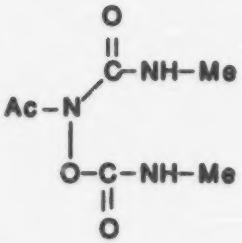
Mouse(iv): LD_{50}: 33700 μg/kg
Cancer Treatment Reports, 64,855,(1980)

Dog(po): LD_{50}: 50 mg/kg
Cancer Treatment Reports, 66,1939,(1982)

Dog(iv): LD_{50}: 6250 μg/kg
Cancer Treatment Reports, 64,855,(1980)

CARACEMIDE

NSC- 253272



Chemical Name:
N-Acetyl-N-(methylcarbamoyloxy)-N'- methylurea

Other Name:
Caracemide (USAN)

Molecular Formula: $C_6H_{11}N_3O_4$ **M.W.:** 189.2

Approximate Solubility:	(mg/ml)
H_2O	> 76
Methanol	> 100
Chloroform	> 100

Stability:

Bulk:
The half life at 45° C. is estimated at 8 weeks and the time for 10% decomposition is 2 weeks.

The compound is stable at room temperature for 4 weeks as determined by HPLC.

Solution:
A 50 mg/ml solution in water at room temperature showed 5% decomposition after 4 hours and 17% decomposition after 24 hours as indicated by HPLC.

Ultraviolet Absorption:

(0.1 N HCl)

The spectrum shows end absorption only.

High Performance Liquid Chromatography:

Column: µBondapak C18, 300 x 3.9 mm ID

Mobile Phase: 20% CH_3OH in H_2O

Flow Rate: 1.0 ml/min

Detection: UV at 210 nm

Sample Preparation: 0.5 mg/ml in internal standard solution

Internal Standard: 0.05 mg aniline in 100 ml methanol

Retention Volumes: 6.0 ml (NSC 253272)
10.0 ml (I.S.)

Toxicity Data:

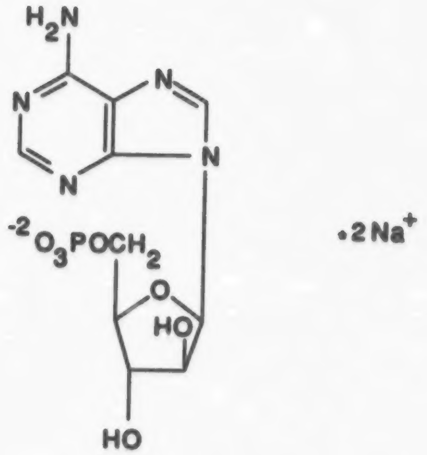
Mouse(po): LD_{50}: 388 mg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 167 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 238 mg/kg
National Technical Information Service, PB84-152032

ARA-AMP DISODIUM SALT

NSC- 259272


H2N
N
N
N
N
-2O3POCH2
O
HO
HO
•2Na+

Chemical Name:
9H-Purin-6-amine, 9-(5-O-phosphono-β-D-arabinofuranosyl)-, disodium salt

Other Names:
Ara-AMP disodium sa[illegible], Vidarabine sodium phosphate

Molecular Formula: $C_{10}H_{12}N_5O_7PNa_2$ **M.W.:** 391.2

BEST COPY AVAILABLE

Approximate Solubility: (mg/ml)

H_2O	> 500
0.1 N NaOH	> 500
0.1 N HCl	> 500
95% EtOH	< 0.05
$CHCl_3$	< 0.05
EtOAc	< 0.05

Stability:

Bulk:
The compound is stable for at least four weeks when stored at room temperature. When stored at 60° C., a gradual decomposition of up to 3% over 4 weeks is observed. (HPLC)

Solution:
As a 10% solution in water at room temperature, the subject compound is stable for at least 9 days as indicated by HPLC.

Ultraviolet Absorption:

(H_2O)

$\lambda_{max} = 260 \pm 2$ nm $\varepsilon = 13{,}500 - 15{,}000$

High Performance Liquid Chromatography:

Column: Spherisorb 10 ODS, 25 cm x 4.6 mm ID

Mobile Phase: 1% dioxane in 0.1 M KH_2PO_4

Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

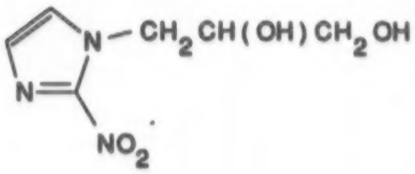
Sample Preparation: 1 mg/ml in internal standard solution

Internal Standard: 1 mg adenosine/ml water

Retention Volume: 3.0 ml (NSC-259272)
9.0 ml (I.S.)

DESMETHYLMISONIDAZOLE

NSC- 261036



Chemical Name:
1,2-Propanediol, 3-(2-nitro-1H-imidazol-1-yl)-

Other Names:
Desmethylmisonidazole; RO 05-9963

Molecular Formula: $C_6H_9N_3O_4$ **M.W.:** 187.2

Approximate Solubility:	(mg/ml)
Water	> 100
Ethanol	40
Methanol	> 100
DMSO	> 100
Acetone	20
Ethyl acetate	6
Chloroform	0.5

Stability:

Bulk:

The bulk chemical is stable for at least 4 weeks when stored at 60° C. as indicated by HPLC.

Solution:

As a 10% solution, the sample is stable at room temperature for at least 5 days, as indicated by HPLC.

Ultraviolet Absorption:

(100% Ethanol)

$\lambda_{max} = 316 \pm 2$ nm $\qquad \varepsilon = 7{,}000 - 7{,}400$

High Performance Liquid Chromatography:

Column: Waters Radial Compression Module C18

Mobile Phase: 3% MeOH in water

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

Sample Preparation: About 0.8 mg/ml in internal standard solution

Internal Standard: 5 mg uracil in 100 ml water

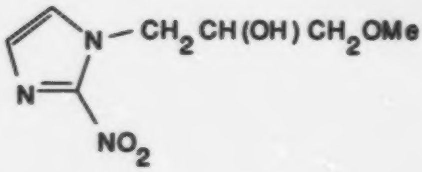
Retention Volumes: 15.0 ml (NSC-261036)
5.5 ml (I.S.)

Toxicity Data:

Mouse(ip): LD_{50}: 2730 mg/kg
Radiation Research, 91,186,(1982)

MISONIDAZOLE

NSC- 261037



Chemical Name:
1H-Imidazole-1-ethanol, α-(methoxymethyl)-2-nitro-

Other Names:
Ro-7-0582; 1-(2-Nitro-Imidazolyl)-3-Methoxy-2-Propanol; Misonidazole

Molecular Formula: $C_7H_{11}N_3O_4$ **M.W.:** 201.2

Approximate Solubility:	(mg/ml)
Water	8
Methanol	70
Ethanol	10
Chloroform	10
Acetone	50
Ethyl acetate	8
Dimethylsulfoxide	> 100
Trifluoroethanol	> 100

Stability:

Bulk:

Protected from light, a sample stored for 90 days at 60° C. showed no decomposition as indicated by UV or TLC. Exposed to light, a sample at room temperature showed 3% decomposition after 90 days.

Solution:

A solution in 0.1 N HCl showed no decomposition after 4 days. As a 2% solution at room temperature with and without light, the compound is also stable for at least 4 days. When kept in the refrigerator for 15 days <1% decomposition occurs. (TLC)

Ultraviolet Absorption:

(95% EtOH)

$\lambda_{max} = 316 \pm 2$ nm $\qquad \varepsilon = 7{,}060 - 7{,}400$

High Performance Liquid Chromatography:

Column: 3.9 mm x 30 cm μBondapak C18

Mobile Phase: 30% MeOH in H_2O

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Retention Volume: 6.0 ml (NSC-261037)

Toxicity Data:

Rat(po): LD_{50}: 2131 mg/kg
National Technical Information Service, PB81-121212

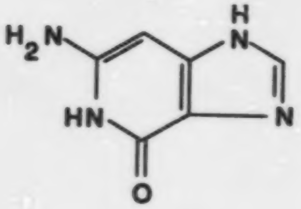
Mouse(po): LD_{50}: 1869 mg/kg
NCI Screening Program Data Summary

Mouse(ip): LD_{50}: 1340 mg/kg
Radiation Research, 91,816,(1982)

Mouse(sc): LD_{50}: 1414 mg/kg
Antimicrobial Agents and Chemotherapy, 513,(1967)

3-DEAZAGUANINE

NSC- 261726



Chemical Name:
4H-Imidazo[4,5-c]pyridin-4-one,6-amino-1,5-dihydro-

Other Names:
3-Deazaguanine; 3-DAG; 3-DG

Molecular Formula: $C_6H_6N_4O$ **M.W.:** 150.1

Approximate Solubility:	(mg/ml)
H_2O	1.9
DMSO	72
Methanol	0.77
Chloroform	0.15

Ultraviolet Absorption:

(0.1 N HCl)

λ_{max}	ε
311 ± 2 nm	6,300 - 6,400
274 ± 2 nm	11,000 - 11,200

High Performance Liquid Chromatography:

Column: Waters RCM 100, C18 cartridge

Mobile Phase: 0.05 M pH 6.6 KH_2PO_4 buffer/CH_3OH, 99/1

Flow Rate: 2.0 ml/min

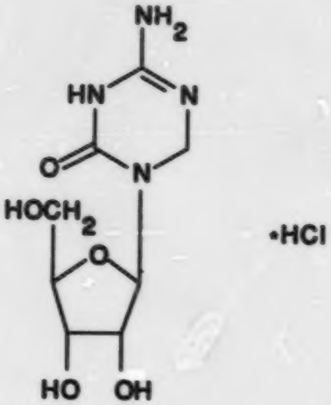
Detection: UV at 254 nm

Sample Preparation: 2.2 mg/ml H_2O

Retention Volume: 14.6 ml (NSC-261726)

DIHYDRO-5-AZACYTIDINE HYDROCHLORIDE

NSC- 264880



Chemical Name:
1,3,5-Triazin-2(1H)-one,4-amino-5,6-dihydro-1-β-D-ribofuranosyl-, monohydrochloride

Other Name:
Dihydro-5-Azacytidine Hydrochloride

Molecular Formula: $C_8H_{14}N_4O_5 \cdot HCl$ **M.W.:** 282.7

Approximate Solubility:	(mg/ml)
H_2O	> 50
pH 4 Acetate buffer	> 50
pH 9 Borate buffer	> 50
10% Ethanol	> 50
95% Ethanol	1 - 3
MeOH	5 - 10
$CHCl_3$	< 1

Stability:

Bulk:

A sample stored at 60° C. for 30 days showed < 1% decomposition as indicated by TLC and UV.

Solution:

A sample was dissolved in pH 8 phosphate buffer at a concentration of 0.1 mg/ml for UV study and 10 mg/ml for TLC study and stored at room temperature in a closed clear bottle exposed to laboratory light for 9 days. Based on the UV and TLC the sample showed < 1% decomposition.

Ultraviolet Absorption:

(pH 9 Phosphate Buffer)

$\lambda_{max} = 234 \pm 2$ nm $\qquad \varepsilon = 6{,}700 - 7{,}100$

High Performance Liquid Chromatography:

Column: Water Associates μBondapak C18, 300 x 3.9 mm ID

Mobile Phase: Water containing 0.005 M heptanesulfonic acid and 1% acetic acid (v/v)

Flow Rate: 2 ml/min

Detection: UV at 234 nm

Sample Preparation: 1 mg/ml in mobile phase containing internal standard.

Internal Standard: 0.063 mg/ml guanosine

Retention Volume: 16.6 ml (NSC - 264880)

Optical Rotation:

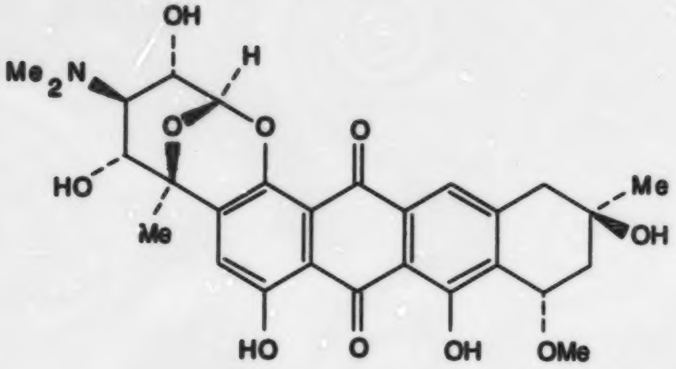
(C = 1.3, H_2O) $[\alpha]^{25}_D = -27.5 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 2559 mg/kg
National Technical Information Service, PB82-195751

MENOGARIL

NSC- 269148



Chemical Name:
2,6-Epoxy-2H-naphthaceno[1,2-b]oxocin-9,16-dione, 4-(dimethylamino)-3,4,5,6,11,12,13,14-octahydro-3,5,8,10,13-pentahydroxy-11-methoxy-6,13-dimethyl-

Other Names:
7-con-O-Methylnogarol; Menogaril (USAN); 7-OMEN

Molecular Formula: $C_{28}H_{31}NO_{10}$ **M.W.:** 541.6

BEST COPY AVAILABLE

Approximate Solubility: (mg/ml)

H_2O	insoluble (< 1 mg/100 ml)
pH 5, 0.1 M Phosphate buffer	insoluble
pH 9, 0.1 M Phosphate buffer	insoluble
95% EtOH	0.05
10% aq. DMA	0.8
DMSO	4
DMA	10

Stability:

Bulk:

Bulk stability studies indicate slight, gradual decomposition occuring over 30 days at room temperature and laboratory illumination; total decomposition was approximated at 2%. Stored at 60° C. and in darkness, the sample is stable for at least 30 days. (HPLC and TLC)

Ultraviolet Absorption:

(95% EtOH)

λ_{max}	ε
478 ± 2 nm	15,000 - 15,200
259 ± 2 nm	23,000 - 24,000
235 ± 2 nm	48,400 - 49,800

High Performance Liquid Chromatography:

Column: Zorbax TMS, 250 mm x 4.6 mm ID

Mobile Phase: 0.1 M KH_2PO_4, pH 5.6/CH_3OH, 45/55

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Retention Volume: 7.1 ml (NSC-269148)

Optical Rotation:

(c = 0.15, $CHCl_3$) $[\alpha]^{21}_D = 920 \pm 13°$

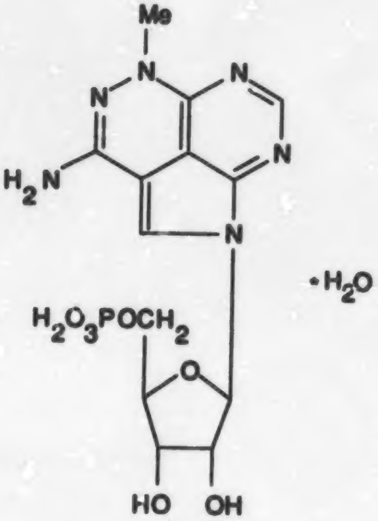
Toxicity Data:

Rat(iv): LD_{50}: 77400 µg/kg
National Technical Information Service, PB84-148410

Mouse(ip): LD_{50}: 83500 µg/kg
National Technical Information Service, PB84-148410

TRICIRIBINE PHOSPHATE

NSC- 280594


Me
N
N
N
N
N
H2N
N
•H2O
H2O3POCH2
O
HO
OH

Chemical Name:

1,4,5,6,8-Pentaazaacenaphthylen-3-amine, 1,5-dihydro-5-methyl-1-(5-O-phosphono-β-D-ribofuranosyl), monohydrate

Other Names:

Tricyclic Nucleoside 5'-Phosphate; Triciribine Phosphate (USAN)

Molecular Formula: $C_{13}H_{17}N_6O_7P{\cdot}H_2O$ **M.W.:** 418.3

Approximate Solubility:	(mg/ml)
MeOH	< 1
DMSO	1 - 5
DMF	< 1
Trifluoroacetic acid	>50
H_2O	< 1
pH 4 Acetate buffer	< 1
pH 9 Borate buffer	1 - 5
pH 9 Carbonate buffer	10 - 15
0.1 N HCl	< 1
10% EtOH	< 1
95% EtOH	< 1

Stability:

Bulk:

A sample stored at 60° C. for 30 days showed no decomposition as indicated by TLC or UV.

Solution:

A solution (.0156 mg/ml) in pH 9 carbonate-bicarbonate buffer showed no decomposition as detected by UV absorption after 9 days.

Ultraviolet Absorption:

(0.1 N NaOH)

$\lambda_{max} = 292 \pm 2$ nm $\qquad \varepsilon = 11{,}700 - 12{,}500$

High Performance Liquid Chromatography:

Column: 300mm x 3.9 mm ID Waters μBondapak C18

Mobile Phase: Methanol/pH 7 0.01 M phosphate buffer with 0.005 M tetrabutylammonium hydroxide 25/75, v/v.

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: pH 9 carbonate buffer containing internal standard

Internal Standard: acetanilide

Retention Volume: 25.6 ml (NSC-280594)

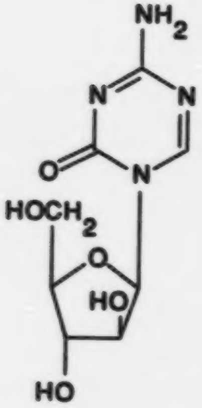
Toxicity Data:

Mouse(ip): LD_{50}: 193 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 109 mg/kg
NCI Screening Program Data Summary

FAZARABINE

NSC- 281272



Chemical Name:
1,3,5-Triazin-2(1H)-one, 4-amino-1-β-D-arabinofuranosyl-

Other Names:
5-Azacytosine arabinoside; ARA-AC, Fazarabine

Molecular Formula: $C_8H_{12}N_4O_5$ **M.W.:** 244.2

Approximate Solubility:	(mg/ml)
Water	> 16
Ethanol	insoluble
Dimethylsulfoxide	> 165

Ultraviolet Absorption:

(95% EtOH)

λ_{max} = 243 ± 2 nm ε = 7,150 - 7,350

High Performance Liquid Chromatography:

Column: Waters RCM 100, C18

Mobile Phase: 0.04 M pH 4.6 KH_2PO_4/CH_3OH, 99/1

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

Sample Preparation: Methanol solution

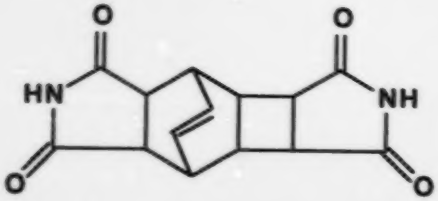
Retention Volume: 16.6 ml (NSC-281271)

Optical Rotation:

(c = 1.2, H_2O) $[\alpha]^{25}_D = 121.5 \pm 2°$

MITINDOMIDE

NSC- 284356



Chemical Name:
4,8-Ethenopyrrolo[3',4':3,4]cyclobut[1,2-f]isoindole-1,3,5,7-(2H,6H)-tetrone, octahydro-

Other Name:
Mitindomide (USAN)

Molecular Formula: $C_{14}H_{12}N_2O_4$ **M.W.:** 272.3

Approximate Solubility: (mg/ml)

p-dioxane	slightly soluble
Aqueous NaOH (2 moles NaOH per mole of compound)	> 20

Stability:

Solution:

A solution was prepared by dissolving 100 mg of drug in 3.0 ml of 0.25 N NaOH. This solution was diluted to 5.0 ml with water to give a final concentration of 20 mg/ml. At room temperature this solution shows 10% decomposition in 40 minutes and 50% decomposition in 5 hours. (HPLC)

Ultraviolet Absorption:

(p-dioxane)

$\lambda_{max} = 252 \pm 2$ nm $\qquad\qquad \varepsilon = 346 - 366$

High Performance Liquid Chromatography:

Column: 300 mm x 4.6 mm ID RP-8

Mobile Phase: 10% CH_3CN in H_2O, pH adjusted to 4 with HOAc

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: A 3.4-mg sampling is quickly dissolved in 1.0 ml of 0.05 N NaOH with the aid of sonication and vigorous mixing. At exactly 1.0 min after addition of the solvent the solution is chromatographed.

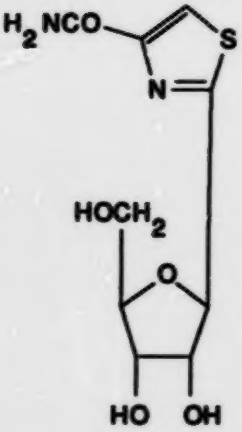
Retention Volume: 8.1 ml (NSC-284356)

Toxicity Data:

Mouse(iv): LD_{50}: 193 mg/kg
NCI Screening Program Data Summary

TIAZOFURIN

NSC- 286193



Chemical Name:
4-Thiazolecarboxamide, 2-β-D-ribofuranosyl-

Other Names:
Tiazofurin (USAN); TCAR; Riboxamide

Molecular Formula: $C_9H_{12}N_2O_5S$ **M.W.:** 260.3

Approximate Solubility:
Soluble in water

Stability:

Bulk:

The compound is stable through 30 days at 60° C. in the dark. (HPLC)

Solution:

In water < 1% decomposition occurs through 24 hours. (HPLC)

Ultraviolet Absorption:

(95% Ethanol)

$\lambda_{max} = 236 \pm 2$ nm $\quad\quad \varepsilon = 7{,}660 - 7{,}970$

High Performance Liquid Chromatography:

Column: Waters μBondapak C18, 300 x 3.9 mm ID

Mobile Phase: Methanol/1% acetic acid in water (10/90, v/v)

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.25 mg/ml in water containing internal standard

Internal Standard: thymidine, 0.3 mg/ml in water

Retention Volume: 5.0 ml (NSC-286193)

Optical Rotation:

(c = 0.914, DMF) $[\alpha]^{25}_D = -13.8 \pm 2°$

Toxicity Data:

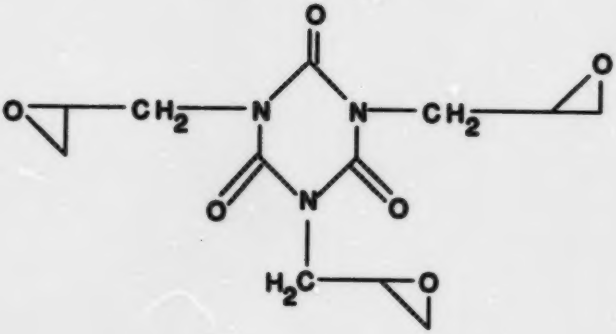
Mouse(ip): LD_{50}: 1684 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 3400 mg/kg
National Technical Information Service, PB83-156901

Dog(iv): LD_{Lo}: 1090 mg/kg
National Technical Information Service, PB83-156901

TEROXIRONE

NSC- 296934



Chemical Name:
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione,
1,3,5-tris(oxiranylmethyl)-, (α)-

Other Names:
Henkel's Compound; Triazinetrione triepoxide; α-Triglycodyl isocyanurate; α-TGI; Teroxirone (USAN)

Molecular Formula: $C_{12}H_{15}N_3O_6$ M.W. : 297.3

Approximate Solubility:	(mg/ml)
Water	< 1
0.1 N HCl	< 1
pH 4 buffer	2.5 - 5
pH 9 buffer	< 1
0.1 N NaOH	1 - 2.5
10% EtOH	< 1
95% EtOH	< 1

Stability:

Bulk:
After heating at 60° C. for 30 days in the dark, the sample purity dropped from > 99% to 93 ± 1%. (HPLC)

Solution:
A solution in water decomposed 29% in 72 hours. When acetonitrile was substituted for water as the storage solvent, < 1% decomposition was observed through 72 hours. (HPLC)

High Performance Liquid Chromatography:

Column: Waters μBondapak C18, 300 x 3.9 mm ID

Mobile Phase: CH_3CN/H_2O, 20/80, v/v

Flow Rate: 1 ml/min

Detection: UV at 205 nm

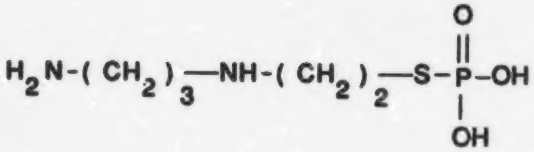
Sample Preparation: 1.0 mg/ml in internal standard solution

Internal Standard: 0.24 µl/ml acetophenone in CH_3CN/H_2O, 20/80,(v/v)

Retention Volumes: 6.4 ml (NSC-296934)
18.5 ml (I.S.)

ETHIOFOS

NSC- 296961



$$H_2N-(CH_2)_3-NH-(CH_2)_2-S-\overset{\overset{O}{\|}}{\underset{\underset{OH}{|}}{P}}-OH$$

Chemical Name:
Ethanethiol, 2-[(3-aminopropyl)amino]-, dihydrogen phosphate (ester)

Other Names:
Amifostine; Gammaphos; WR-2721; Ethiofos (USAN)

Molecular Formula: $C_5H_{15}N_2O_3PS$ M.W. : 214.2

Approximate Solubility:	(mg/ml)
Water	~ 450
95% Ethanol	< 0.01
Chloroform	< 0.01
Toluene	< 0.01

Stability:

Bulk:

A small sample stored in a small container at 60° C. showed about 14% decomposition in 24 hours. A small sample stored in a large container at 60° C. for 30 days appeared to be stable. The stability of the compound is dependent on the temperature and the relative amount of moisture present. (HPLC and TLC)
The compound should be stored under refrigeration in tightly closed containers.

Solution:

A 5% aqueous solution showed about 1% decomposition after 24 hours at room temperature, as indicated by TLC.

High Performance Liquid Chromatography:

Column: C18 Reverse Phase, 300 mm x 4 mm ID

Mobile Phase: H_2O

Flow Rate: 1.0 ml/min

Detection: UV at 200 nm

Sample Preparation: Immediately prior to injection each sampling was dissolved in 0.10 ml of water

Retention Volume: 4.0 ml (NSC-296961)

Toxicity Data:

Rat(ip): LD_{50}: 418 mg/kg
Radiobiologiya, 16,249,(1976)

Rat(im): LD_{50}: 396 mg/kg
Radiobiologiya, 16,249,(1976)

Mouse(po): LD_{50}: 842 mg/kg
Radiobiologiya, 20,746,(1980)

Mouse(ip): LD_{50}: 321 mg/kg
NCI Screening Program Data Summary

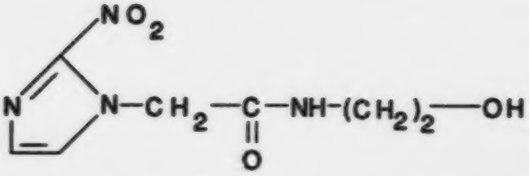
Mouse(iv): LD_{50}: 557 mg/kg
National Technical Information Service, PB81-199580

Mouse(im): LD_{50}: 514 mg/kg
Radiobiologiya, 16,249,(1976)

Dog(iv): LD_{Lo}: 279 mg/kg
Toxicologic Pathology, 13,58,(1985)

SR-2508

NSC- 301467



Chemical Name:
1H-Imidazole-1-acetamide, N-(2-hydroxyethyl)-2-nitro-

Other Name:
SR 2508

Molecular Formula: $C_7H_{10}N_4O_4$ M.W. : 214.2

Approximate Solubility:	(mg/ml)
Water	> 100
Methanol	60
Ethanol	30
Chloroform	< 1

Stability:

Bulk:
The sample is stable at room temperature for at least one month. (HPLC)

Solution:

As a 10% solution in water, the chemical is stable for at least 24 hours. (HPLC)

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 323 \pm 2$ nm $\varepsilon = 7{,}540 - 8{,}020$

High Performance Liquid Chromatography:

Column: 3.9 mm x 30 cm μBondapak C18

Mobile Phase: 100% H_2O

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg/ml in internal standard solution

Internal Standard: 8.6 mg uracil/100ml H_2O

Retention Volume: 8.6 ml (NSC-301467)
5.6 ml (I.S.)

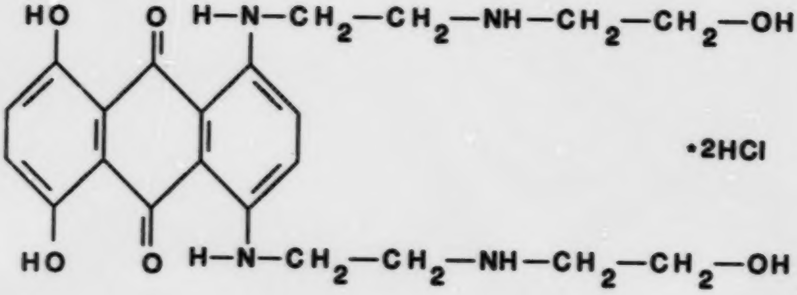
Toxicity Data:

Mouse(ip): LD_{50}: 3300 mg/kg
Radiation Research, 91,186,(1982)

Mouse(iv): LD_{50}: 4400 mg/kg
International Journal of Radiation Oncology, Biology and Physics, 12,1097(1986)

MITOXANTRONE HYDROCHLORIDE

NSC- 301739



Chemical Name:
9,10-Anthracenedione, 1,4-dihydroxy-5,8-bis[[2-[(2-hydroxyethyl)amino]ethyl]amino]-, dihydrochloride

Other Names:
CL 232,315; DHAQ; DHAD; Dihydroxyanthracenedione dihydrochloride; Mitoxantrone Hydrochloride (USAN)

Molecular Formula: $C_{22}H_{28}N_4O_6{\cdot}2HCl$ M.W. : 517.4

Approximate Solubility:	(mg/ml)
H_2O	5 - 10
pH 4 Acetate buffer	3 - 5
pH 9 Borate buffer	< 1
0.1 N HCl	1 - 3
0.1 N NaOH	decomposes
10% Ethanol	3 - 5
95% Ethanol	< 1
Methanol	< 1

Stability:

Bulk:

After 30 days at 60° C., no decomposition was observed. (UV or TLC)

Solution:

The solution undergoes 6% decomposition in H_2O through 5 days as judged by UV.

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
670 ± 2 nm	25,230 - 25,270
617 ± 2 nm	19,850 - 19,930
277 ± 2 nm	13,360 - 13,400
241 ± 2 nm	40,000 - 40,920

High Performance Liquid Chromatography:

Column: µPhenyl Porasil, 300 x 4 mm ID

Mobile Phase: CH_3OH/1.5% acetic acid in H_2O with 0.005 M heptanesulfonic acid, 50/50, v/v

Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

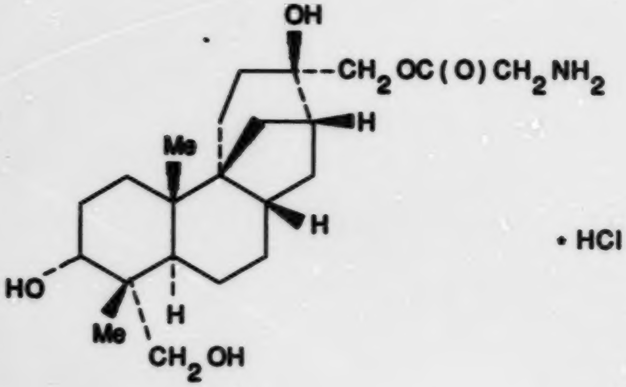
Sample Preparation: Sample solvent - CH_3OH/pH 4
acetate buffer, 25/75, v/v

Internal standard: hexaphenone 15 µl/l sample solvent.

Retention Volume: 16.5 ml (NSC-301739)
36 ml (I.S.)

APHIDICOLIN GLYCINATE

NSC - 303812



Chemical Name:
Glycine, (tetradecahydro-3,9-dihydroxy-4-(hydroxymethyl)-4,11b-dimethyl-8,11a-methano-11aH-cyclohepta(a)naphthalen-9-yl)methyl ester, hydrochloride, (3R-(3α,4α,4aα,6aβ,8β,9β,11aβ,11bβ)-

Other Names:
Aphidicolin glycinate;aphidicolin-17-glycinate;
ICI 137233

Molecular Formula: $C_{22}H_{37}NO_5 \cdot HCl$ M.W. 432.0

BEST COPY AVAILABLE

Approximate Solubility:	(mg/ml)
H_2O	100
MeOH	100
$CHCl_3$	< 0.001

Stability:

Bulk:
Compound is stable at 25 ± 2° C. under normal illumination or in the dark and at 45° C. for at least 4 weeks, as determined by HPLC.

Solution:
An 8 mg/ml solution in water at room temperature (25 ± 2° C.) decomposes at an apparent linear rate of 0.20 ± 0.05% per hour over a 24 hr period.

Ultraviolet Absorption: Exhibits end absorption only.

High Performance Liquid Chromatography:

Column: Zorbax Sil, 250 x 4.6 mm (I.D.)

Mobile Phase: $CH_3CN/CH_3OH/NH_4OH$ (conc.), 160/40/0.1

Flow Rate: 1 ml/min

Detection: UV at 206 nm

Sample Preparation: 5 mg in 1 ml CH_3OH 8 µl injection volume

Internal Standard: thymine

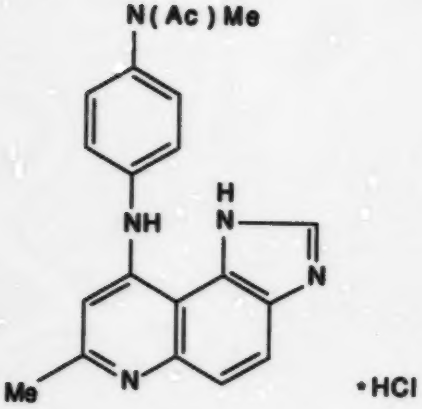
Retention Volume: 6.3 ml

Optical Rotation:

(c = 1, MeOH) $[\alpha]^{20}_{D} = +4.5 \pm 0.5°$

ACODAZOLE HYDROCHLORIDE

NSC- 305884



Chemical Name:
Acetamide, N-methyl-N-[4-[(7-methyl-1-H-imidazo(4,5-*f*) quinolin-9-yl)amino]phenyl]-, monohydrochloride

Other Name:
Acodazole Hydrochloride (USAN)

Molecular Formula: $C_{20}H_{19}N_5O{\cdot}HCl$ M.W. : 381.9

Approximate Solubility:	(mg/ml)
H_2O	> 50
pH 4 Acetate buffer	> 50
pH 9 Carbonate buffer	> 50
10% Ethanol	> 50
Methanol	10-12
95% Ethanol	10-15
0.1 N HCl	> 50
0.1 N NaOH	< 1

Stability:

Bulk:
The bulk compound does not undergo significant decomposition when heated at 60° C. for 30 days in the dark. (HPLC) The compound is quite hygroscopic.

Solution:
A solution (0.1 mg/ml) prepared in unbuffered water and stored at room temperature and exposed to light is stable for > 48 hours. (HPLC)

Ultraviolet Absorption: (corrected for water content)

(Methanol)

λ_{max}	ε
345 ± 2 nm	15,300 - 16,600
316 ± 2 nm	12,400 - 13,200
255 ± 2 nm	27,900 - 30,500
227 ± 2 nm	21,100 - 22,400

High Performance Liquid Chromatography:

Column: Waters µBondapak C18, 300 x 3.9 mm ID

Mobile Phase: Methanol/water (containing 2%
acetic acid), 40/60 (v/v)

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Retention Volume: 11.6 ml (NSC-305884)

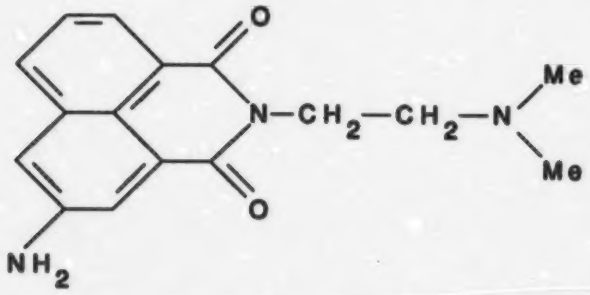
Toxicity Data:

Mouse(ip): LD_{50}: 161 mg/kg
NCI Screening Program Data Summary

Mouse(iv): LD_{50}: 87,590 µg/kg
NCI Screening Program Data Summary

AMONAFIDE

NSC - 308847



Chemical Name:
1H-Benz[de]isoquinoline-1,3(2H)-dione, 5-amino-2-[2-(dimethylamino)ethyl]-

Other Names:
Nafidimide , Amonafide

Molecular Formula: $C_{16}H_{17}N_3O_2$ **M.W.:** 283.3

Approximate Solubility:	(mg/ml)
H_20	< 1
pH 4 acetate buffer	~ 10
pH 9 carbonate buffer	< 1
0.1 N HCl	~ 20
0.1 N NaOH	< 1
10 % Ethanol	< 1
95 %	5-7
Methanol	5-7

Stability:

Bulk:

A sample stored at 60° C. for 30 days assayed at >99% by HPLC.

Solution:

A 0.4 mg/ml solution of drug in 0.2 M Acetate buffer (pH4.0) showed no decomposition after 48 hrs at room temperature as indicated by HPLC.

High Performance Liquid Chromatography:

Column: Waters, µ Bondapak C18, 300 x 3.9 mm ID.

Mobile Phase: CH_3CN/0.005 M Heptanesulfonic acid adjusted to pH 2.5 with H_2SO_4, 32/68,v/v.

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.04 mg/ml in CH_3CN/0.005 M Heptanesulfonic acid adjusted to pH 2.5 with H_2SO_4 (5/75,v/v) containing internal standard

Internal Standard: Indole, 0.2 mg/ml

Retention Volume: 8.3 ml (NSC 308847)
20.1 ml (I.S.)

Ultraviolet Absorption:

(MeOH)

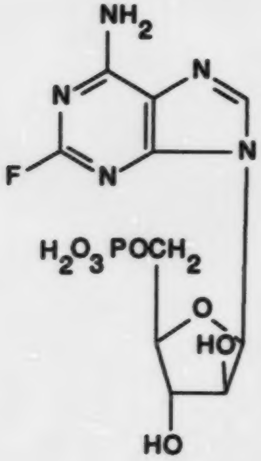
λ_{max}	ε
217 ± 2nm	27,200 - 29,400
249 ± 2nm	26,000 - 27,200
342 ± 2nm	8,050 - 8,450
422 ± 2nm	4,200 - 4,400

Toxicity Data:

Mouse(iv): LD_{50}: 69 mg/kg
National Technical Information Service, PB84-219542

FLUDARABINE PHOSPHATE

NSC- 312887



Chemical Name:
9H-Purin-6-amine, 2-fluoro-9-(5-O-phosphono-β-D-arabinofuranosyl)-

Other Names:
Fludarabine Phosphate (USAN); 2-F-ARA AMP; 2-Fluoro-Adenine Arabinoside-5'-phosphate; 2-Fluoro-ARA AMP

Molecular Formula: $C_{10}H_{13}FN_5O_7P$ **M.W. : 365.2**

Approximate Solubility:	**(mg/ml)**
Water	9.2
pH 4 buffer	27.6
pH 9 buffer	57

Stability:

Bulk:
Based on HPLC analysis, the sample is stable for at least one month when stored as the bulk chemical at room temperature and 60° C.

Solution:
A 2-mg/ml aqueous solution is stable for at least 48 hours at room temperature and laboratory illumination. (HPLC)

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 262 \pm 2$ nm $\varepsilon = 12{,}600 - 13{,}400$

High Performance Liquid Chromatography:

Column: Alltech ODS, 250 x 4.6 mm ID

Mobile Phase: 5% MeOH in 0.1 M KH_2PO_4 buffer, pH 4

Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.2 mg/ml in internal standard solution

Internal Standard: 0.3 mg thymidine/ml water

Retention Volume: 13.0 ml (NSC-312887)
19.5 ml (I.S.)

Optical Rotation:

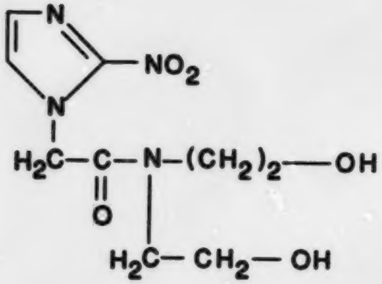
(C = 0.5, H_2O) $[\alpha]^{21}_D = 12 \pm 2°$

Toxicity Data:

Mouse(iv): LD_{50}: 1236 mg/kg
National Technical Information Service, PB83-195685

SR-2555

NSC- 314055


N
NO2
N
H2C—C—N—(CH2)2—OH
O
H2C—CH2—OH

Chemical Name:
1H-Imidazole-1-acetamide, N,N-bis(2-hydroxyethyl)-2-nitro-

Other Name:
SR-2555

Molecular Formula: $C_9H_{14}N_4O_5$ **M.W. :** 258.2

Approximate Solubility:	(mg/ml)
Water	> 100
Methanol	> 100
Ethanol	78
Chloroform	< 1

Ultraviolet Absorption:

(MeOH)

λ_{max} = 314 ± 2 nm ε = 7,430 - 7,470

High Performance Liquid Chromatography:

Column: 3.9 mm x 30 cm μBondapak C18

Mobile Phase: Water

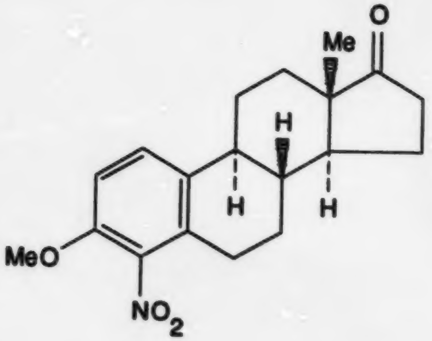
Flow Rate: 1.5 ml/min

Detection: UV at 254 nm

Retention Volume: 15.0 ml (NSC-314055)

4-NITROESTRONE

NSC - 321803



Chemical Name:
Estra-1,3,5[10]-trien-17-one, 3-methoxy-4-nitro-

Other Name:
4-Nitroestrone, methyl ether

Molecular Formula: $C_{19}H_{23}NO_4$ M.W. 329.4

BEST COPY AVAILABLE

Approximate Solubility:	**(mg/ml)**
H_20	< 0.66
Buffer, pH 4	< 0.65
Buffer, pH 9	< 0.65
Ethanol	0.69 - 0.73
DMA	≥ 11.60
DMSO	4.27 - 6.41
$CHCl_3$	≥ 11.60
Ethyl acetate	4.60 - 9.20
t-Butanol	< 0.65
THF	5.16 - 10.30
CH_3CN	5.02 - 10.00
DMSO/H_2O (60%)	< 0.66
DMA/H_2O (10%)	< 0.66
EtOH/H_2O (10%)	< 0.66

Stability:

Bulk:

A sample stored at 50° C. for 3 months showed no decomposition as indicated by HPLC.

Solution:

A 0.06 mg/ml solution of drug in 60% DMSO/H_2O at room temperature showed 10% drug decomposition in 5.41 hours as determined by HPLC.

Ultraviolet Absorption:

(Acetonitrile)

λ_{max}	ε
254 ± 2 nm	1,100 - 1,400
275 ± 2 nm	1,577 - 1,700

High Performance Liquid Chromatography:

Column: μ Bondapak C-18, 300 x 3.9 nm ID

Mobile Phase: 55% CH_3CN in H_2O

Flow Rate: 2 ml/min

Detection: UV at 254 nm

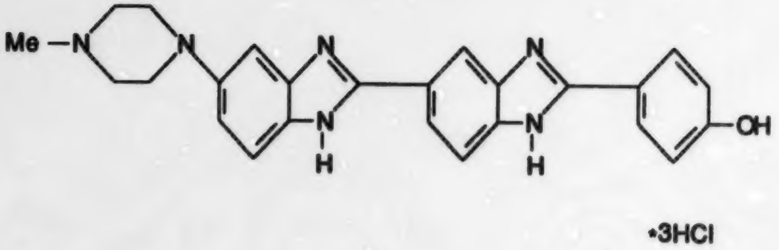
Sample Preparation: 4.0 mg/ml of sample, 0.32 mg/ml internal standard in dimethylacetamide

Internal Standard: Norgestrel

Retention Volume: 23.0 ml (NSC 321803)
11.1 ml (I.S.)

PIBENZIMOL HYDROCHLORIDE

NSC- 322921



Chemical Name:
Phenol, 4-[5-(4-methyl-1-piperazinyl)-[2,5'-bi-1H-benzimidazol]-2'-yl]-, trihydrochloride

Other Names:
Bisbenzimidazole; Pibenzimol Hydrochloride

Molecular Formula: $C_{25}H_{24}N_6O \cdot 3HCl$ M.W. : 534.9

Approximate Solubility:	(mg/ml)
DMSO	240 - 300
H_2O	~ 110
95% EtOH	< 1
0.1 N NaOH	14 - 22
0.1 N HCl	43 - 44
$CHCl_3$	< 1
Acetone	< 1

Stability:

Bulk:

As a bulk chemical in a capped-glass vial maintained at room temperature and under ordinary laboratory illumination, the material slowly decomposes. At the end of four weeks under these conditions, 3% decomposition has occurred. (HPLC) In a similar container but maintained at 45° C. and in darkness, the subject sample is stable for at least four weeks. (HPLC)

Solution:

A solution of the sample (1 mg/ml) is stable in water for at least 24 hours at room temperature under normal laboratory illumination. (HPLC)

High Performance Liquid Chromatography:

Column: Dupont Zorbax ODS, 25 cm x 4.6 mm ID

Mobile Phase: 0.1 M pH 7.0 KH_2PO_4/CH_3OH, 88/200

Flow Rate: 1.5 ml/min

Detection: UV at 230 nm

Sample Preparation: 1 mg/ml in H_2O

Retention Volume: 10.95 ml (NSC-322921)

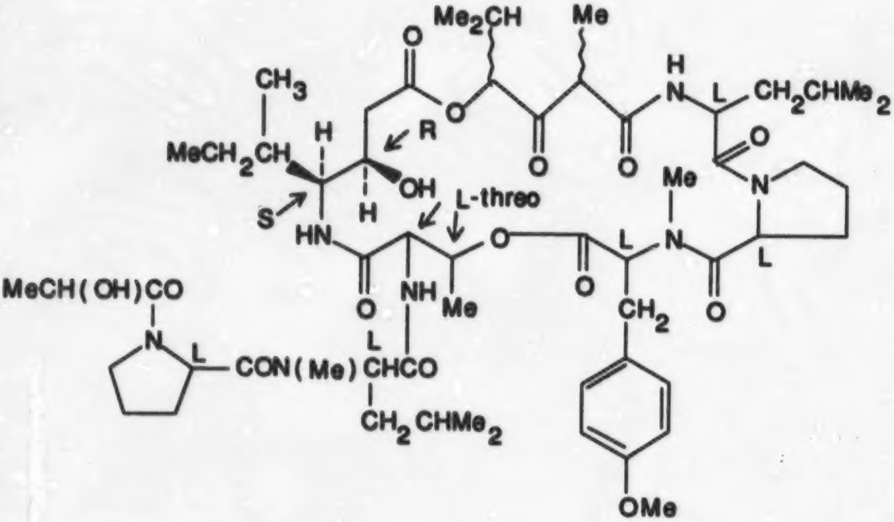
Toxicity Data:

Rat(iv): LD_{50}: 32200 µg/kg
National Technical Information Service, PB84-171206

Mouse(iv): LD_{50}: 36900 µg/kg
National Technical Information Service, PB84-171206

DIDEMNIN B

NSC- 325319


Me2CH
Me
O
CH3
H
H
N
L
CH2CHMe2
O
R
MeCH2CH
O
O
O
Me
N
OH
S
H
L-threo
HN
O
O
L
N
L
MeCH(OH)CO
O
NH
Me
O
CH2
O
N
L
L
CON(Me)CHCO
CH2CHMe2
OMe

Name:
Didemnin B

Molecular Formula: $C_{57}H_{89}N_7O_{15}$ **M.W. : 1112.0**

Approximate Solubility:	**(mg/ml)**
H_2O	< 0.1
CH_3OH	> 100
$CHCl_3$	> 100
DMSO	> 100
C_2H_5OH	> 100
CH_2Cl_2	> 100

BEST COPY AVAILABLE

Stability:

Bulk:

As a bulk chemical, didemnin B is found to be stable at 25 ± 2° C. for 3 weeks. At the end of 4 weeks, approximately 2% decomposition has occurred.

When stored at 45° C., didemnin B appeared stable for 2 weeks; after this time, it slowly decomposed to an approximate 7% loss at the end of 4 weeks. (HPLC)

Solution:

As a 6 mg/ml 50% aqueous ethanol solution at room temperature (25 ± 2° C.), didemnin B appeared stable for at least 26 hours. (HPLC)

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
284 ± 2 nm(sh)	1,455 - 1,490
277 ± 2 nm	1,705 - 1,750
220 ± 2 nm(sh)	17,500 - 19,199
205 ± 2 nm	29,100 - 29,700

High Performance Liquid Chromatography:

Column: 250 mm x 4.6 mm ID, Whatman Partisil 5 ODS

Mobile Phase: CH_3OH/H_2O/triethylamine, 75/25/0.01
(adjusted to pH 7.5 with acetic acid)

Flow Rate: 1.0 ml/min

Detection: UV at 275 nm

Sample Preparation: 3 mg/ml in internal standard solution

Internal Standard: 1 ml hexaphenone per liter methanol

Retention Volumes: 19 ml (NSC-325319)
10 ml (I.S.)

Toxicity Data:

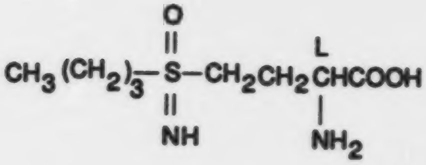
Rat(iv): LD_{50}: 860 µg/kg
National Technical Information Service, PB84-192251

Mouse(iv): LD_{50}: 1530 µg/kg
National Technical Information Service, PB84-192251

Dog(iv): LD_{Lo}: 418 µg/kg
National Technical Information Service, PB84-192251

BSO

NSC - 326231



$$CH_3(CH_2)_3-\underset{\underset{NH}{\|}}{\overset{\overset{O}{\|}}{S}}-CH_2CH_2\underset{\underset{NH_2}{|}}{\overset{L}{C}}HCOOH$$

Chemical Name:
Butanoic acid, 2-amino-4-(S-butylsulfonimidoyl)-

Other Names:
L-Buthionine sulfoxime; BSO

Molecular Formula: $C_8H_{18}N_2O_3S$ **M.W.:** 222.3

Approximate Solubility:	**(mg/ml)**
H_2O	> 100
Acetate buffer, pH4	> 100
Carbonate buffer, pH9	> 100
0.1 N HCl	> 100
0.1 N NaOH	> 100
MeOH	< 1
EtOH (95%)	< 1
CH_3CN	< 1
EtOAC	< 1
$CHCl_3$	< 1
Dimethylacetamide	< 1
DMSO	< 1

Stability:

Bulk:

Samples subjected to both light and dark conditions at room temperature showed no decomposition after 90 days. Samples kept at 50° C. in both light and dark conditions showed about 1 % decomposition after 90 days.

Solution:

BSO was found to be stable in aqueous solution for 72 hours when stored at room temperature and under laboratory light.

Ultraviolet Absorption:

(H_2O)

No absorbance was observed between 220-420 nm.

High Performance Liquid Chromatography:

Column: Alltech Econosphere C18, 5μ, 250 x 4.6 mm I.D.

Mobile Phase: 0.01 M Phosphate buffer, pH 5.0

Flow Rate: 1.0 ml/min

Detection: UV at 205 nm

Sample Preparation: Samples were prepared in distilled H_2O to give concentrations of approximately 0.57 mg/ml.

Internal Standard: Thymine (0.006 mg/ml in distilled H_2O)

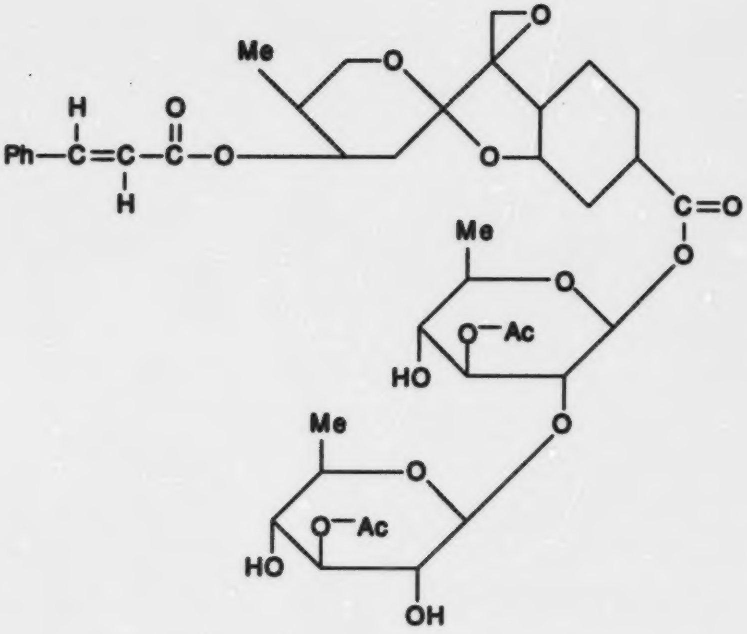
Retention Volume: 8.0 ml (NSC - 326231)

Optical Rotation:

(c = 1, 1N HCl) $[\alpha]^{22}_{D} = +32.5 \pm 2°$

PHYLLANTHOSIDE

NSC- 328426


Me
O
O
H
O
Ph—C=C—C—O
H
O
C=O
Me
O
O
O—Ac
HO
O
Me
O
O—Ac
HO
OH

Chemical Name:
β-D-Glucopyranose, 2-O-(3-O-acetyl-6-deoxy-, 3-acetate 1-[decahydro-5''-methyl-4''-[1(oxo-3-phenyl-2-propenyl)oxy]dispiro[oxirane-2,3''(2'H)-benzofuran-2,2''-[2H]pyran]-6'-carboxylate, [2S-[2α[4R*(E),5'S*],3β,3aα,6α,7aα]]-

Other Name:
Phyllanthoside

Molecular Formula: $C_{40}H_{52}O_{17}$ M.W. : 804.8

Approximate Solubility:	(mg/ml)
H_2O	< 0.1
C_2H_5OH	> 100
$CHCl_3$	> 100
DMSO	> 100
CH_3OH	> 100
CH_2Cl_2	> 100

Stability:

Bulk:
The bulk compound is stable for at least four weeks at room temperature and 45° C. (HPLC)

Solution:
The room temperature stability in 10% aqueous ethanol (1 mg/ml) shows t_{90} to be 1.5 hours and t_{50} to be 19 hours. (HPLC)

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
276 ± 2 nm	20,450 - 20,730
216 ± 2 nm	15,370 - 15,970
205 ± 2 nm	13,820 - 14,670

High Performance Liquid Chromatography:

Column: 300 mm x 3.9 mm ID Waters μ-Porasil

Mobile Phase: $CH_2Cl_2/CH_3OH/H_2O$ (96/4/0.4)

Flow Rate: 0.8 ml/min

Detection: UV at 254 nm

Sample Preparation: One mg of sample is dissolved in 1 ml CH_2Cl_2.

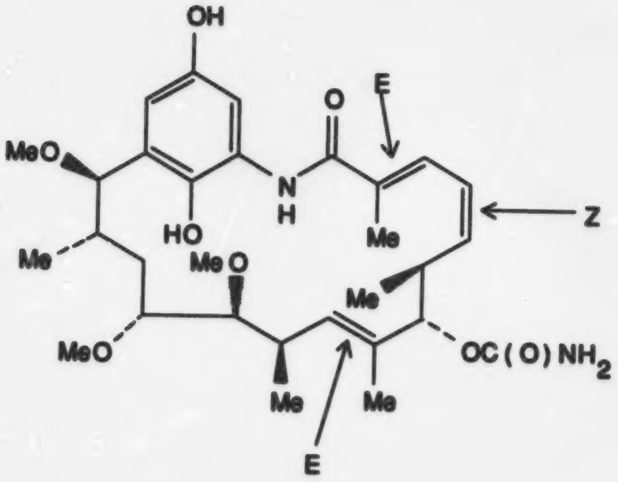
Retention Volume: 11.6 ml (NSC-328426)

Optical Rotation:

($C = 0.7$, $CHCl_3$) $[\alpha]^{20}_D = 17.7 \pm 2°$

MACBECIN II

NSC- 330500



OH
O
E
MeO
N
H
Z
HO
Me
Me
Me O
Me
MeO
OC (O) NH2
Me
Me
E

Chemical Name:
Geldanamycin,18,21-didehydro-6,17-didemethoxy-18,21-dideoxo-18,21-dihydroxy-15-methoxy-6-methyl-11-O-methyl-, (6S,15R)-

Other Name:
Macbecin II

Molecular Formula: $C_{30}H_{44}N_2O_8$ M.W. : 560.8

BEST COPY AVAILABLE

Approximate Solubility: (mg/ml)

H_2O	< 0.1
0.1 N NaOH	unstable
0.1 N HCl	< 0.1
0.1 M phosphate buffer, pH 9	< 0.1
95% EtOH	7
Acetone	7
MeOH	40
DMSO	> 100
$CHCl_3$	< 0.1

Stability:

Bulk:

As a bulk chemical, Macbecin II is stable for at least 4 weeks under ordinary laboratory conditions. At 45° C. the material gradually decomposes. The time for 10% decomposition is approximately 3 weeks. (HPLC)

Solution:

A 2 mg/ml solution in 95% ethanol at room temperature shows 10% decomposition in 26 hours. The major decomposition product is a quinone form of Macbecin II. (HPLC)

High Performance Liquid Chromatography:

Column: 3.9 mm ID x 30 cm μBondapak C18

Mobile Phase: 60% MeOH/40% H_2O

Flow Rate: 2 ml/min

Detection: UV at 254 nm

Retention Volume: 9.2 ml (NSC-330500)

Optical Rotation:

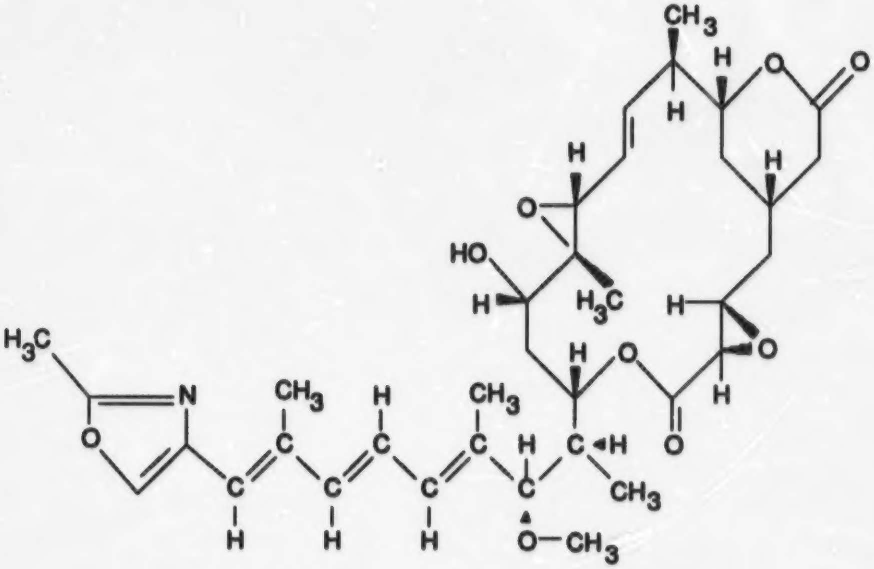
(c = 0.5%, MeOH) $[\alpha]^{20}_{D} = +58 \pm 2°$

Toxicity Data:

Mouse(ip): LD_{50}: 25 mg/kg
Journal of Anhtibiotics, 33,205,(1980)

RHIZOXIN

NSC - 332598



Name:
Rhizoxin

Molecular Formula: $C_{35}H_{47}NO_9$ **M.W.:** 625.8

Approximate Solubility:	**(mg/ml)**
H_2O	< 1
MeOH	> 50
$CHCl_3$	> 50

BEST COPY AVAILABLE

Stability:

Bulk:

HPLC analysis indicated that the bulk chemical is unstable under both light and dark conditions at room temperature and at 50° C. Freezer storage is recommended.

Solution:

The compound is unstable in a solution of DMF/H_2O (40/60,v/v) through 72 hrs. The t_{90} was 5.2 hrs.

Ultraviolet Absorption:

(~8 µg/ml in MeOH)

λ_{max}	ε
323 ± 2nm	39,750 ± 540
309 ± 2nm	53,260 ± 620
297 ± 2nm	42,240 ± 595

High Performance Liquid Chromatography:

Column: Alltech Econosphere C18, 5µ. 250 x 4.6 mm ID

Mobile Phase: CH_3CN/pH 7 phosphate buffer, 0.01 M (55/45,v/v)

Flow Rate: 1.0 ml/min

Detection: UV at 280 nm

Sample Preparation: 11.77 mg of compound was diluted with eluent to give test sample concentrations of about 1, 0.2 and 0.02 mg/ml.

Internal Standard: Phenanthrene, 0.01 mg/ml in eluent

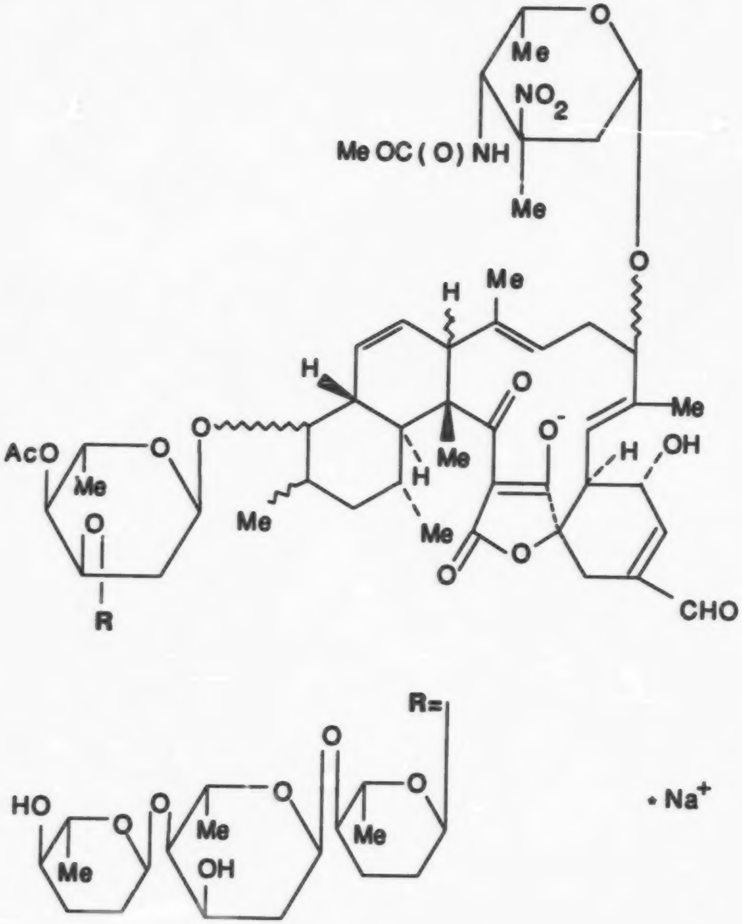
Retention Volume: 10.4 ml (NSC - 332598)

Optical Rotation:

($c = 0.5, CH_3OH$) $[\alpha]^{23}_{D} = +160 \pm 4°$

TETROCARCIN A, SODIUM SALT

NSC- 333856


Me
NO2
MeOC(O)NH
Me
O
H
Me
H
O
AcO
O
Me
O
R
Me
Me
H
Me
O-
OH
H
O
O
CHO
Me
R=
HO
O
Me
O
Me
OH
O
O
Me
• Na+

Names:

Tetrocarcin A, sodium salt; Antlermicin A, monosodium salt

BEST COPY AVAILABLE

Molecular Formula: $C_{67}H_{95}N_2O_{24}\cdot Na$ M.W. : 1335.5

Approximate Solubility:	(mg/ml)
H_2O	> 100
MeOH	> 100
95% EtOH	> 100
DMSO	> 100
0.1 N HCl	< 0.1
0.1 N NaOH	~ 5
$CHCl_3$	~ 0.6

Ultraviolet Absorption:

(90% MeOH)

$\lambda_{max} = 265 \pm 2$ nm ε = 11,400 - 11,800

High Performance Liquid Chromatography:

Column: Ultrasphere ODS 5 µm, 4.6 mm x 250 mm

Mobile Phase: 70% MeOH in 0.1 M NaOAc and 0.01 M citric acid

Flow Rate: 1.2 ml/min

Detection: UV at 254 nm

Sample Preparation: ~1 mg sample is dissolved in 1 ml $MeOH:H_2O$, 1:1 or internal standard solution

Internal Standard: 0.1 mg N-ethylcarbazole/ml MeOH

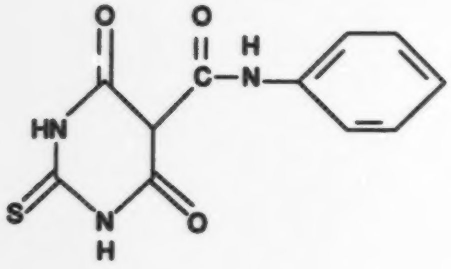
Retention Volumes: 15.6 ml (NSC-333856)
25.2 ml (I.S.)

Optical Rotation:

(C = 1, 10% 0.1 N HCl-90% MeOH) $[\alpha]^{23}_{D} = -63.5 \pm 1°$

MERBARONE

NSC - 336628



Chemical Name:
5-Pyridinecarboxamide, hexahydro-4,6-dioxo-N-phenyl-2-thioxo-

Other Name:
Merbarone

Molecular Formula: $C_{11}H_9N_3O_3S$ **M.W.:** 263.3

Approximate Solubility:	(mg/ml)
H_2O	< 0.1
C_2H_5OH	< 0.1
0.1N HCl	< 0.1
DMSO	80
0.1N NaOH	5
$CHCl_3$	< 0.1
CH_3CN	< 0.1
pH 9 buffer	< 0.1
$(CH_3)_2CO$	< 0.1
TFA	< 0.1
THF	6

Stability:

Bulk:

As a bulk chemical, Merbarone is found to be stable at 25 and 45° C. for at least 4 weeks as determined by HPLC.

Solution:

As a 1 mg/ml pH 9 buffered solution at room temperature (25 ± 2 ° C.), Merbarone appeared stable for at least 24 hrs as determined by HPLC.

Ultraviolet Absorption:

(0.1N NaOH)

λ_{max}	ε
306 ± 2nm	29,600 - 30,300
243 ± 2nm	17,000 - 17,500

High Performance Liquid Chromatography:

Column: Hamilton PRP-1, 250 x 4.1 mm ID

Mobile Phase: 14% CH_3CN in 0.1 M Na_2HPO_4 (pH adjusted to 10.2 with NaOH)

Flow Rate: 1.5 ml/min

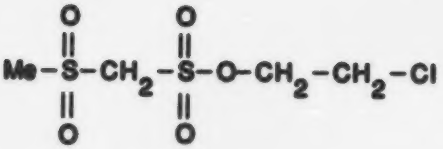
Detection: UV at 243 nm

Sample Preparation: Approximately 1 mg of sample dissolved in 2 ml of mobile phase plus one drop of 5N NaOH

Retention Volume: 7.3 ml (NSC-336628)

CLOMESONE

NSC-338947



$$\mathrm{Me-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-CH_2-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-O-CH_2-CH_2-Cl}$$

Chemical Name:
Methanesulfonic acid, (methylsulfonyl)-, 2-chloroethyl ester

Other Name:
Clomesone

Molecular Formula: $C_4H_9ClO_5S_2$ **M.W.:** 236.7

Approximate Solubility:	(mg/ml)
Water	4
Acetate buffer, pH 4	6
Carbonate buffer, pH 9	6
0.1 N HCl	4
0.1 N NaOH	15
Ethanol (95%)	18
Methanol	> 50
Acetonitrile	> 50
DMSO	> 50

Stability:

Bulk:

Clomesone is stable at room temperature in light or dark conditions but is unstable when stored at 50° C. in both light and dark conditions.

Solution:

The t_{90} of an aqueous solution is 207 minutes.

High Performance Liquid Chromatography:

Column: Altex Ultrasphere ODS, 5 μ, 250 x 4.6 mm ID

Mobile Phase: CH_3CN/0.067 M phosphate buffer, pH 7.0 (25/75, v/v)

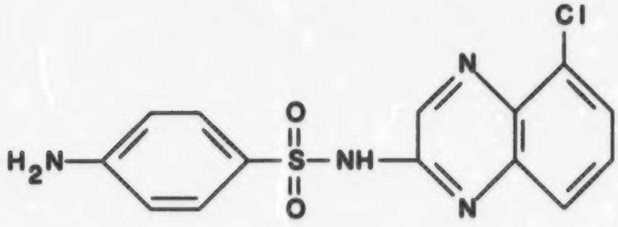
Flow Rate: 1.0 ml/min

Detection: Refractive index

Sample Preparation: Sample was dissolved in
CH_3CN/0.067 M phosphate buffer, pH 7.0 (25/75, v/v)

CHLOROQUINOXALINE SULFONAMIDE

NSC - 339004



Chemical Name:
Benzenesulfonamide, 4-amino-N-(5-chloro-2-quinoxalinyl)-

Other Names:
Chloroquinoxaline sulfonamide

Molecular Formula: $C_{14}H_{11}ClN_4O_2S$ **M.W.:** 334.8

Approximate Solubility: (mg/ml)

H_2O	< 1
pH 4 Acetate buffer	< 1
pH 9 Carbonate buffer	10-12
0.1N HCl	< 1
0.1N NaOH	~ 25 - 30
MeOH	5 - 7
EtOH (95%)	4 - 6
DMSO	> 50

Stability:

Bulk:

The compound is stable at room temperature and ordinary laboratory illumination for at least 90 days. In a capped glass vial and heated at 50° C., the compound is stable for at least 90 days.(HPLC)

Solution:

Dilute solutions (0.8 mg/ml) in 50% DMSO were stable for up to 72 hrs as determined by UV.

Ultraviolet Absorption:

λ_{max}	ε
339 ± 2 nm	5,820 ± 300
269 ± 2 nm	26,730 ± 1,200
255 ± 2 nm	31,000 ± 2,200

High Performance Liquid Chromatography:

Column: Alltech Econosphere C18, 5μ, 250 x 4.6 mm ID

Mobile Phase: CH_3CN/water containing 0.005 M heptanesulfonic acid and sulfuric acid to adjust pH to 3.0, 30/70, v/v.

Flow Rate: 1.0 ml/min

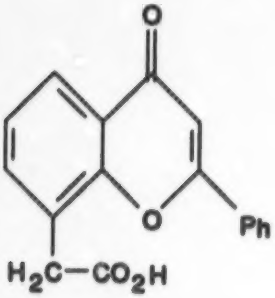
Detection: UV at 254 nm

Sample Preparation: 0.08 mg/ml in CH_3CN

Retention Volume: 15.8 ml (NSC-339004)

FLAVONE ACETIC ACID

NSC - 347512



Chemical Name:
4H-1- Benzopyran-8-acetic acid, 4-oxo-2-phenyl-

Other Name:
Flavone-8-acetic acid

Molecular Formula: $C_{17}H_{12}O_4$ **M.W.:** 280.3

Approximate Solubility: (mg/ml)

Water	< 0.1
0.1N NaOH	~ 20
0.1N HCl	< 0.1
0.1M $NaHCO_3$	< 0.3
95% EtOH	1
MeOH	1
$CHCl_3$	< 0.1
DMSO	> 100
TFA	> 100
10% DMSO	< 1

Stability:

Bulk:
As a bulk chemical, Flavone-8-acetic acid is stable for at least 3 months at 60° C. as determined by HPLC.

Solution:
Solutions of 1 mg/ml dissolved in 0.1N NaOH (pH 9) showed no decomposition for at least 27 hrs.

High Performance Liquid Chromatography:

Column: Varian, C18, 5µm, 150 x 4 mm ID

Mobile Phase: MeOH/H_2O/HAc (55/45/0.05)

Flow Rate: 1.0 ml/min

Detection: UV at 254 nm

Sample Preparation: Approximately 0.25 mg/ml is dissolved in internal standard solution

Internal Standard: m-Nitroaniline (0.15 mg/ml in MeOH)

Retention Volume: 10.4 ml (NSC 347512)

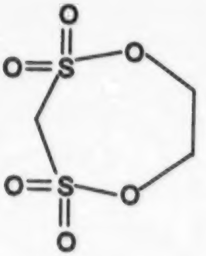
Ultraviolet Absorption:

(95% EtOH)

λ_{max}	ε
296 ± 2nm	21,200 - 21,800
256 ± 2nm	19,000 - 20,300

CYCLODISONE

NSC- 348948



Chemical Name:
1,5,2,4-Dioxadithiepane, 2,2,4,4-tetraoxide

Other Name:
Cyclic-SOSO; cyclodisone

Molecular Formula: $C_3H_6O_6S_2$ **M.W.:** 202.2

Approximate Solubility:	(mg/ml)
Water	< 1
Acetate buffer, pH 4	< 1
Carbonate buffer, pH 9	< 1
0.1 N HCl	< 1
0.1 N NaOH	10-13
Ethanol (95%)	< 1
Acetone	> 100
CH_3CN	> 100
$CHCl_3$	< 1
DMSO	> 100
DMF	> 100

Stability:

Bulk:

Cyclodisone stored for 90 days at room temperature and at 50° C. under both dark and light conditions was stable with respect to drug composition. Samples stored at 50° C. turned a light tan color.

Solution:

180 mg of Cyclodisone was dissolved in 60 ml of DMSO/water (50/50,v/v). Aliquots of this solution (5 ml) were diluted to 10 ml with internal standard solution (5 ml, phenol 1.8 mg/ml in CH_3CN/water, 20/80, v/v) and the concentration was determined over a 4 hour period using the HPLC system described below. The t_{90} was 320 min.

High Performance Liquid Chromatography:

Column: Altech Ultrasphere ODS, 5μ, 250 x 4.6 mm ID

Mobile Phase: CH_3CN/water (20/80,v/v)

Flow Rate: 1.0 ml/min

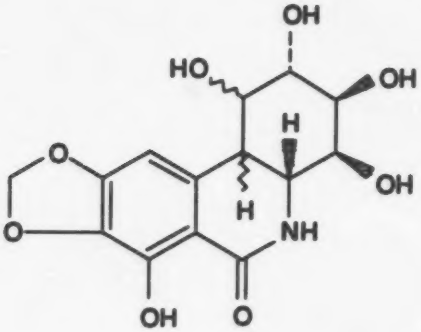
Detection: Refractive index

Sample Preparation: 1.7 mg/ml in CH_3CN/H_2O (20/80,v/v)

Retention Volume: 7.6 ml (NSC-348948)

PANCRATISTATIN

NSC - 349156



Name:
Pancratistatin

Molecular Formula: $C_{14}H_{15}NO_8$ **M.W.:** 325.3

Approximate Solubility:	(mg/ml)
H_2O	< 1
Acetate buffer (pH4)	< 1
Carbonate buffer (pH9)	< 1
0.1N HCl	< 1
0.1N NaOH	~ 5-7
MeOH	< 1
95% EtOH	< 1
10% EtOH	< 1
$CHCl_3$	< 1
DMF	10-15

BEST COPY AVAILABLE

Stability:

Bulk:

The bulk drug was determined to be stable at 60° C. under both light and dark conditions for 30 days as determined by HPLC.

Solution:

Pancratistatin was stable in 50% DMSO/H_20 for 24 hr as determined by HPLC.

Ultraviolet Absorption:

(0.1N NaOH)

λ_{max}	ε
332 ± 2nm	4,000 - 4,100
280 ± 2nm	5,700 - 6,000
233 ± 2nm	23,800 - 24,800

High Performance Liquid Chromatography:

Column: Waters μBondapak C18, 10μ, 300 x 3.9 mm ID

Mobile Phase: CH_3CN/HOAc (10/90, v/v)

Flow Rate: 1.0 ml/min

Detection: UV at 280 nm

Sample Preparation: Sample is dissolved in DMSO to give a concentration of ~0.65 mg/ml. Internal standard concentration is 0.2 mg/ml.

Internal Standard: Theophylline (1.035 mg/ml in DMSO).

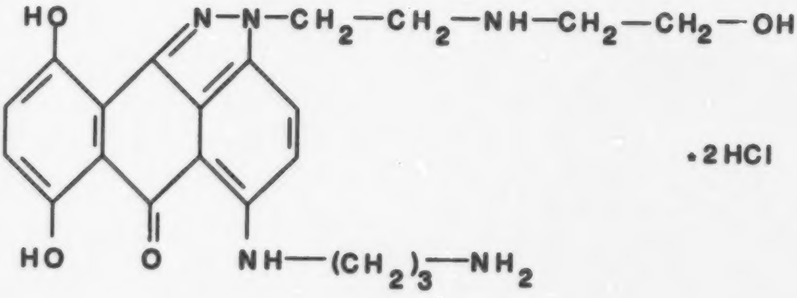
Retention Volume: 18.3 ml (NSC 349156)
8.6 ml (I.S.)

Optical Rotation:

(C = 1, H_2O) $[\alpha]^{25}_D = +44 \pm 2°$

OXANTRAZOLE

NSC - 349174


HO
N
N
CH2
CH2
NH
CH2
CH2
OH
•2HCl
HO
O
NH
(CH2)3
NH2

Chemical Name:
Anthra[1,9-cd]pyrazol-6(2H)-one,
5-[3-(aminopropyl)amino]-7,10-dihydroxy-
2-[2-[(2-hydroxyethyl)amino]ethyl]-, dihydrochloride

Other names:
Anthrapyrazole derivative; Oxantrazole

Molecular Formula: $C_{21}H_{25}N_5O_4{\cdot}2HCl$ **M.W.:** 484.4

Approximate Solubility:	(mg/ml)
H_2O	> 11.2
Buffer, pH4	> 9.6
Buffer, pH9	> 11.5
Ethanol	< 0.73
DMA	< 0.70
DMSO	> 9.6
$CHCl_3$	< 0.77
EtOAc	< 0.71
t-BuOH	< 0.71

Stability:

Bulk:

Samples stored at 25° C. under both light and dark conditions and at 50° C. in the dark for three months showed no significant degradation as determined by HPLC.

Solution:

A solution containing 10.2 mg/ml in water showed approximately 5% degradation in 24 hr. The test sample exhibited <10% degradation in 48 hr.

Ultraviolet Absorption:

(H_2O)

λ_{max}	ε
254 ± 2nm	10,358 ± 500
295 ± 2nm	6,146 ± 400
318 ± 2nm	6,889 ± 400
333 ± 2nm	6,677 ± 400
406 ± 2nm	4,827 ± 400
515 ± 2nm	16,592 ± 600

High Performance Liquid Chromatography:

Column: Zorbax C-8, 250 x 4.6 mm I.D., with a 5µ RP-8 guard column, 30 x 4.6 mm I.D.

Mobile Phase: 5% CH_3CN/20 % DMF water(0.2M ammonium acetate/L mobile phase, adjusted with HAc to pH 4.5.)

Flow Rate: 1 ml/min

Detection: UV at 254 nm

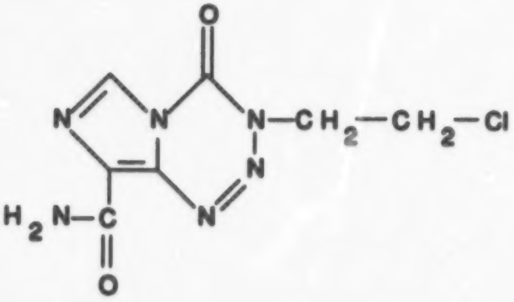
Sample Preparation: 10 mg [illegible] sample diluted to 10 ml with internal standard solution

Internal Standard: 1.0 mg/ml benzamide in water.

Retention Volume: 11.14 ml (NSC - 349174)
6.17 ml (I.S.)

MITOZOLOMIDE

NSC - 353451



Chemical Name:
Imidazo[5,1,-d]-1,2,3,5-tetrazine-8-carboxamide,
3-(2-chloroethyl)-3,4-dihydro-4-oxo-

Other Names:
Mitozolamide; Azolastone

Molecular Formula: $C_7H_7ClN_6O_2$ **M.W.:** 242.5

Approximate Solubility:	**(mg/ml)**
H_2O	0.0
Buffer, pH 4	0.0
Buffer, pH 9	≤ 0.7
EtOH	0.0
DMA	≤ 4.9
DMSO	≤ 5.1
$CHCl_3$	≤ 0.7
EtOAc	0.0
t-BuOH	0.0
90% BuOH	≤ 0.8
Ether	0.0
THF	≤ 2.0

High Performance Liquid Chromatography:

Column: RCM-100, 10 µm C-18, 100 x 8 mm I.D.

Mobile Phase: 10% CH_3CN/water containing 0.005M sodium heptanesulfonate, pH adjusted to 3 with HAc.

Flow Rate: 2.0 ml/min

Detection: UV at 254 nm

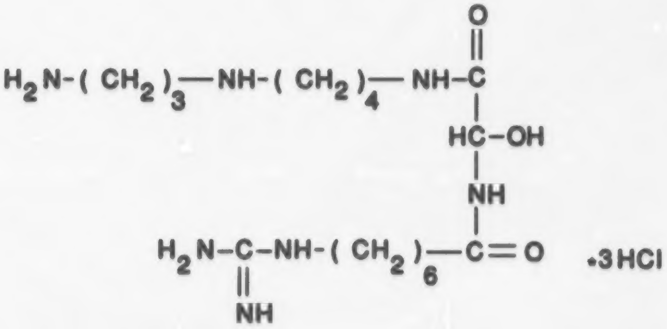
Sample Preparation: 8.0 mg sample diluted to 5 ml with internal standard solution.

Internal Standard: 3-(2-hydroxyethyl)-1,2,3-benzotriazinone (2.0 mg/ml in DMSO).

Retention Volume: 13.7 ml (NSC - 353451)
20.5 ml (I.S.)

DEOXYSPERGUALIN

NSC - 356894



Chemical Name:
Heptanamide, 7-[(aminoiminomethyl)amino]-N-[2-[[4-[(3-aminopropyl)amino]butyl]amino]-1-hydroxy-2-oxoethyl]-, (+)-, trihydrochloride

Other Name: 15-Deoxyspergualin trihydrochloride

Molecular Formula: $C_{17}H_{37}N_7O_3 \cdot 3HCl$ **M.W.:** 496.9

Approximate Solubility:	(mg/ml)
H_2O	> 100
0.1N NaOH	> 100
0.1N HCl	> 100
95% EtOH	> 100
MeOH	> 100
DMSO	> 100
$CHCl_3$	< 0.2

Stability:

Bulk:

Samples stored at 25° C. for 3 months show 5-8% decomposition as determined by HPLC.

Solution:

As a 2 mg/ml solution in water at 25° C., 15-deoxyspergualin is stable for at least 28 hrs under ordinary laboratory conditions as determined by HPLC.

Ultraviolet Absorption:

(95% EtOH)

The spectrum shows end absorption only.

High Performance Liquid Chromatography:

Column: Ultrasphere ODS, 220 x 4.6 mm I.D.

Mobile Phase: 10% CH_3CN in 0.1 M KH_2PO_4 and 0.005 M hexanesulfonic acid sodium salt, pH adjusted to 3 with H_3PO_4

Flow Rate: 1.0 ml/min

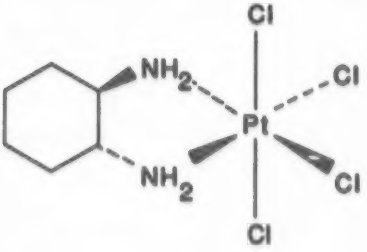
Detection: UV at 205 nm

Sample Preparation: Approximately 1 mg/ml in water.

Retention Volume: 4.2 ml (NSC-356894)

TETRAPLATIN

NSC - 363812



Chemical Name:
Platinum, tetrachloro(1,2-cyclohexanediamine-N,N')-, [OC-6,22-(trans)]-

Other Name:
Tetraplatin

Molecular Formula: $C_6H_{14}Cl_4N_2Pt$ **M.W.:** 451.1

Approximate Solubility:	(mg/ml)
H_2O	5.0 - 10.0

BEST COPY AVAILABLE

Stability:

Bulk:

Samples stored at 25° C. in the dark or under laboratory illumination for 90 days or at 50° C. in the dark for 90 days showed no appreciable degradation.

Solution:

The compound is unstable in aqueous solutions but is stable in normal saline for more than 24 hrs.

Ultraviolet Absorption:

λ_{max}

266 ± 2 nm
254 ± 2 nm
210 ± 2 nm

High Performance Liquid Chromatography:

Column: Zorbax C8, 250 x 4.6 mm with Perisorb RP-8 guard column

Mobile Phase: water

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.4 mg/ml (0.9% NaCl)

Internal Standard: thymine

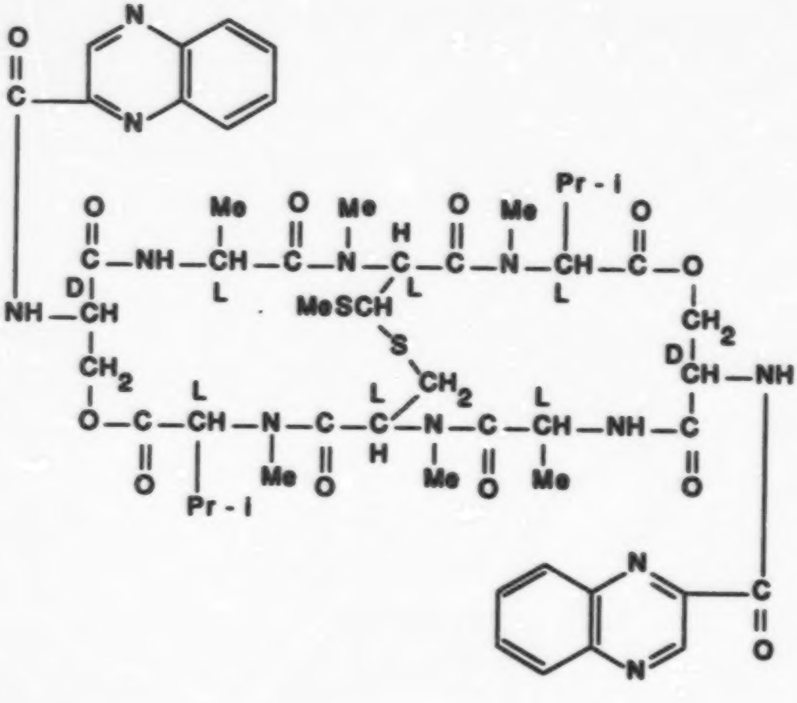
Retention Volume: 7.6 ml (NSC-363812)

Toxicity Data:

Mouse(iv): LD_{50}: 10 mg/kg
Cancer Treatment Reports, 61,1519,(1977)

ECHINOMYCIN

NSC- 526417



Name:
Echinomycin

Other Name:
Quinomycin A

Molecular Formula: $C_{51}H_{64}N_{12}O_{12}S_2 \cdot H_2O$ M.W. : 1119.3

BEST COPY AVAILABLE

Approximate Solubility:

Soluble in 5% Cremophor EL : 5% ethanol: 90% water at 0.4 mg/ml. Very insoluble in water.

Stability:

Bulk:

Should be stored at 5° C. or less.

Ultraviolet Absorption:

(Methanol)

λ_{max}	ε
321 ± 2nm	12,500 - 13,500
243 ± 2nm	73,400 - 77,400

High Performance Liquid Chromatography:

Column: Waters 10 μBondapak C18, 300 x 3.9 mm ID

Mobile Phase: Acetonitrile/water, 60/40 (v/v)

Flow Rate: 1 ml/min

Detection: UV at 254 nm

Sample Preparation: 0.5 mg/ml in acetonitrile

Retention Volume: 5.8 ml (NSC-526417)

Optical Rotation:

(C = 1.10, chloroform) $[\alpha]^{23}_{D} = -321 \pm 2°$

Toxicity Data:

Mouse(ip): LD_{50}: 400 µg/kg
Antibiotics: Origin, Nature and Properties, 1,311,(1978)

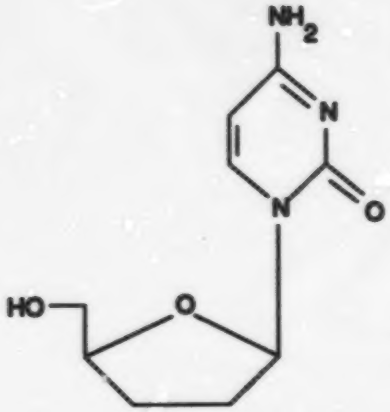
Mouse(sc): LD_{50}: 3800 µg/kg
Antibiotics: Origin, Nature and Properties, 1,311,(1978)

Mouse(iv): LD_{50}: 629 µg/kg
National Technical Information Service, PB83-114298

Dog(iv): LD_{Lo}: 89 µg/kg
National Technical Information Service, PB83-114298

DIDEOXYCYTIDINE

NSC - 606170



Chemical Name:
2',3'-Dideoxycytidine

Other Names:
Dideoxycytidine; DDC

Molecular Formula: $C_9H_{13}N_3O_3$ **M.W.:** 211.2

Approximate Solubility:	(mg/ml)
H_2O (warm)	80-90
Acetate buffer, pH 4	> 50
Carbonate buffer, pH 9	> 50
0.1N HCl	> 50
0.1N NaOH	> 50
EtOH (95%)	5-7
MeOH	8-10
BuOH	< 1
DMA	7-10
DMSO	90-100
DMSO (70%)	50-60
CH_3CN	< 1
EtOAc	< 1
$CHCl_3$	< 1
Toluene	< 1

Stability:

Bulk:
Dideoxycytidine is stable in bulk form through 90 days at room temperature and at 50° C. under both light and dark conditions.

Solution:
Dideoxycytidine is stable in distilled water through 72 hrs.

Ultraviolet Absorption:

(0.1 N HCl)

$\lambda_{max} = 280 \pm 2nm$ $\varepsilon = 13,300 \pm 700$

High Performance Liquid Chromatography:

Column: Alltech Econosphere, 300 x 3.9 mm I.D.

Mobile Phase: 0.2 M Ammonium acetate, pH 7.0

Flow Rate: 1 ml/min

Detection: UV at 280 nm

Sample Preparation: Approximately 10 mg (accurately weighed) is dissolved in 50 ml water. Four ml of this solution is added to 2 ml of internal standard solution and the resulting solution is diluted to 10 ml with distilled water.

Internal Standard: 5-Bromo-2'-deoxyuridine, ~0.5 mg/ml in methanol/water, 5/45, v/v.

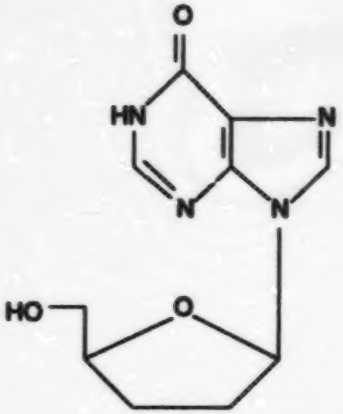
Retention Volumes: 37 ml (NSC 606170)
51 ml (I.S.)

Optical Rotation:

(C = 1, H_2O) $[\alpha]^{25}_{D} \geq +70°$

DIDEOXYINOSINE

NSC - 612049



Chemical Name:
2',3' Dideoxyinosine

Other Names:
Dideoxyinosine; DDI

Molecular Formula: $C_{10}H_{12}N_4O_3$ **M.W.:** 236.2

Approximate Solubility:	(mg/ml)
H_2O	20
0.1 N KH_2PO_4 (pH4)	19
0.1N KH_2PO_4 (pH9)	23
MeOH	5
EtOH	2.5
DMSO	43
$CHCl_3$	insoluble

Stability:

Bulk:
The compound is stable for at least 6 weeks at room temperature and 45° C. under both light and dark conditions.

Solution:
The compound is stable as a 0.5 mg/ml aqueous solution for more than 24 hrs under normal laboratory conditions.

Ultraviolet Absorption:

λ_{max}	ε
203 ± 2nm	18,400 – 19,970
249 ± 2nm	12,200 – 12,500

High Performance Liquid Chromatography:

Column: IBM ODS, 250 x 4.6 mm (I.D.)

Mobile Phase: 10% MeOH/0.1N KH_2PO_4, pH = 6.8

Flow Rate: 1.3 ml/min

Detection: UV at 254 nm

Sample Preparation: 1 mg DDI dissolved in 2 ml water

Retention Volume: 14.7 ml

Optical Rotation:

(C = 1, H_2O) $[\alpha]^{20}_{D} = -25.7 \pm 2°$

INDEX

Drug Name	NSC Number	Page Number
Acetamide, N,N-Hexamethylenebis	95580	69
Acivicin	163501	138
Aclacinomycin A Hydrochloride	208734	159
Aclarubicin Hydrochloride	208734	159
Acodazole Hydrochloride	305884	226
Acridinyl Anisidide	249992	176
Actinomycete Fermentation Product	135758	114
Adriamycin Hydrochloride	123127	91
L-Alanosine, monosodium salt	153353	135
Alpha-TGdR	71851	56
Alpha-2'-Deoxythioguanosine	71851	56
Altretamine	13875	29
Amethopterine	740	1
Amifostine	296961	214
4-Amino-10-Methylfolic Acid	740	1
2-Amino-1,3,4-Thiadiazole	4728	18
Amonafide	308847	229
AMSA	249992	176
Amsacrine	249992	176
Anguidine	141537	120
Anthrapyazole derivative	349174	276
Antlermicin A, monosodium salt	333856	258
Aphidicolin Glycinate	303812	223
ARA-AC	281272	203
ARA-AMP disodium salt	259272	183
AT-125	163501	138
Azacitidine	102816	77
5-Azacytidine	102816	77

INDEX

Drug Name	NSC Number	Page Number
5-Azacytosine arabinoside	281272	203
Aziridinylbenzoquinone	182986	150
AZQ	182986	150
BA-163	45383	53
Bisbenzimidazole	322921	240
Bromodeoxyuridine	38297	44
Bruceantin	165563	141
BSO	326231	246
BUdR	38297	44
Buthionine Sulfoximine	326231	246
Caracemide	253272	180
Carboplatin	241240	170
Calcium Leucovorin	3590	15
CBDCA	241240	170
Chloroquinoxaline Sulfonamide	339004	266
Cis-Diamminedichloroplatinum(II)	119875	87
Cisplatin	119875	87
Citrovorum Factor	3590	15
CL 232,315	301739	220
Clomesone	338947	264
7-con-O-Methylnogarol	269148	197
Co-Vidarabine	218321	162
CPD	119875	87
Crystalline Antibiotic	135758	114
Cyclo-C	145568	129
Cyclocytidine Hydrochloride	145668	129
Cyclodisone	348948	271
DAG	132313	105
3-DAG	261726	192

INDEX

Drug Name	NSC Number	Page Number
Daunomycin Hydrochloride	82151	59
Daunorubicin Hydrochloride	82151	59
DDA	98700	72
3-Deazauridine	126849	97
3-Deazaguanine	261726	192
Delta-9-Tetrahydrocannabinol	134454	111
Delta-9-THC	134454	111
2'-Deoxycoformycin	218321	162
Deoxyspergualin	356894	281
Desmethylmisonidazole	261036	186
3-DG	261726	192
DHAQ	301739	220
Diacetoxyscirpenol	141537	120
1,2:5,6-Dianhydrogalactitol	132313	105
Diaziquone	182986	150
Dichloromethotrexate	29630	37
Didemnin B	325319	243
Dideoxyadenosine	98700	72
Dideoxycytidine	606170	289
Dideoxyinosine	612049	292
Diglycoaldehyde	118994	84
Dihydro-5-Azacytidine	264880	194
Dihydrotriazine benzenesulfonyl fluoride	127755	100
Dihydroxyanthracenedione Dihydrochloride	301739	220
DON	7365	21
Doxorubicin Hydrochloride	123127	91
Ebifuramin	201047	156

INDEX

Drug Name	NSC Number	Page Number
Echinomycin	526417	286
Emofolin Sodium	139490	117
Ethiofos	296961	214
Fazarabine	281272	203
Flavone Acetic Acid	347512	268
Fludarabine Phosphate	312887	232
2-Fluoro-Adenine Arabinoside 5'-phosphate	312887	232
2-Fluoro-ARA-AMP	312887	232
5-Fluoro-1(Tetrahydro-2-Furyl)-Uracil	148958	132
Folinic Acid	3590	15
FT-203	148958	132
Ftorafur	148958	132
Gammaphos	296961	214
Guanazole	1895	9
Henkel's Compound	296934	211
Hexamethylmelamine	13875	29
HMBA	95580	69
Homoharringtonine	141633	123
HXM	13875	29
N-(2-Hydroxyethyl)-2-Nitro-1H-Imidazole-1-Acetamide	301467	217
ICRF-159	129943	103
ICRF-187	169780	144
Idoxuridine	39661	47
Imidazole-1-Acetamide	301467	217
Indicine N-Oxide	132319	108
Inosine Dialdehyde	118994	84

INDEX

Drug Name	NSC Number	Page Number
Inox	118994	84
5-Iododeoxyuridine	39661	47
5-IUDR	39661	47
JB-11 (Acetate Salt)	249008	173
Ladakamycin	102816	77
Leucovorin Calcium	3590	15
Macbecin II	330500	252
m-AMSA	249992	176
Melphalan	8806	23
Menogaril	269148	197
Merbarone	336628	261
Mercaptopurine	755	7
6-Mercaptopurine	755	7
Methotrexate	740	1
Methyl CCNU	95441	63
N-Methylformamide	3051	12
Methyl GAG	32946	40
Methyl-G	32946	40
Methylglyoxal Bisguanylhydrazone Dihydrochloride Monohydrate	32946	40
6-Methylmercaptopurine Riboside	40774	50
6-Methyl MP-riboside	40774	50
5-Methyltetrahydrohomofolate	139490	117
Misonidazole	261037	189
Mitindomide	284356	205
Mitoguazone Dihydrochloride	32946	40
Mitoxantrone Hydrochloride	301739	220
Mitozolomide	353451	279
6-MMPR	40774	50
5-MTHHF	139490	117

INDEX

Drug Name	NSC Number	Page Number
MTX	740	1
Nafidimide	308847	229
4-Nitroestrone	321803	237
7-OMEN	269148	197
Oxantrazole	349174	276
PALA Disodium	224131	165
L-PAM	8806	23
Pancratistatin	349156	273
PC-501	45383	53
PCNU	95466	66
Pentamethylmelamine Hydrochloride	118742	81
Pentostatin	218321	162
Phenylalanine Mustard	8806	23
N-Phosphonoacetyl-L-Aspartate Disodium	224131	165
Phyllanthoside	328426	249
2,5-Piperazinedione, 3,6-Bis-(5-Chloro-2-Piperidyl)-, Dihydrochloride	135758	114
Pibenzimol Hydrochloride	322921	240
Prednisolone Sodium Succinate	9151	26
Purine-6-Thiol, Monohydrate	755	7
Quinomycin A	526417	286
Rapamycin	226080	167
Razoxane	129943	103
Rhizoxin	332598	255
RO 05-9963	261036	186
RO-7-0582	261037	189

INDEX

Drug Name	NSC Number	Page Number
Rubidomycin Hydrochloride	82151	59
Sangivamycin HCl	143648	126
L-Sarcolysin	8806	23
Semustine	95441	63
Spirogermanium Hydrochloride	192965	153
Spiromustine	172112	147
Spiro-32	192965	153
SR 2508	301467	217
SR-2555	314055	235
Streptonigrin	45383	53
Taxol	125973	94
TCAR	286193	208
Tegafur	148958	132
Teroxirone	296934	211
Tetraplatin	363812	283
Tetrocarcin A, sodium salt	333856	258
6-TG	752	4
α-TGI	296934	211
THC	134454	111
Thioguanine	752	4
6-Thioguanine	752	4
Thymidine	21548	34
Tiazofurin	286193	208
TMCA	36354	42
Triazinetrione Triepoxide	296934	211
Triciribine Phosphate	280594	200
Tricyclic Nucleoside 5'-Phosphate	280594	200
α-Triglycodyl Isocyanurate	296934	211

INDEX

Drug Name	NSC Number	Page Number
Uridine	20256	32
U-42126	163501	138
Vidarabine sodium phosphate	259272	183
WR-2721	296961	214
Wyeth WY-5321	118994	84
Yoshi-864	102627	75

★ U.S. GOVERNMENT PRINTING OFFICE: 1989— 201-778/80332

NIH Publication No. 88-2654
August 1988

303